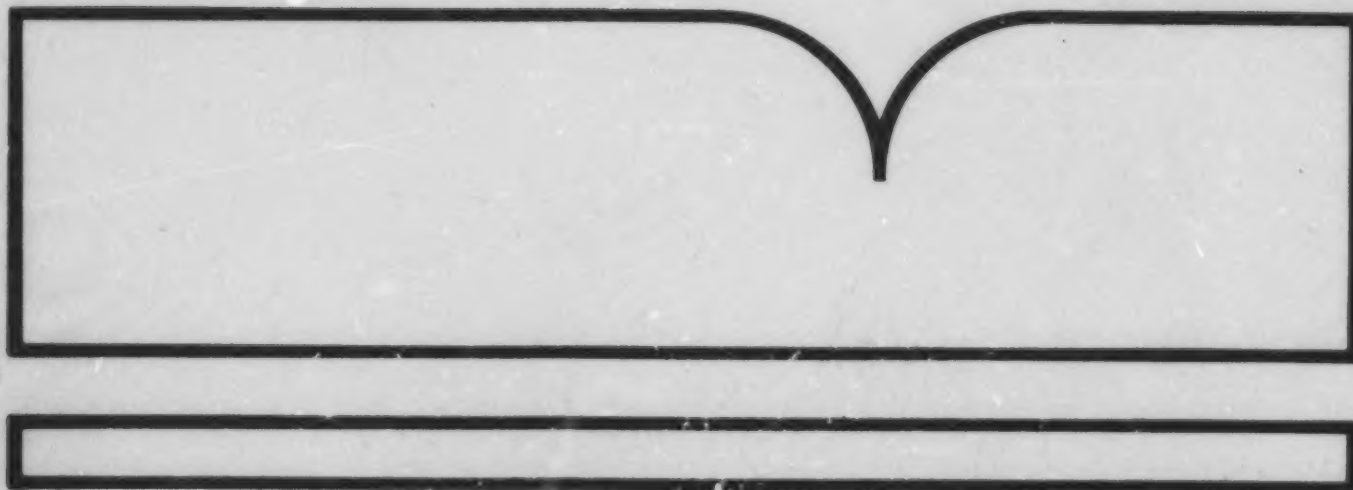


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Dispersion Modeling Techniques in Estimating
Short-Term Sulfur Dioxide Concentrations

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AN EVALUATION OF ALTERNATIVE GAUSSIAN
PLUME DISPERSION MODELING TECHNIQUES
IN ESTIMATING SHORT-TERM SULFUR DIOXIDE
CONCENTRATIONS

by

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AUTHOR'S AFFILIATION

The author was an employee of the National Oceanic and Atmospheric Administration, U. S. Department of Commerce on assignment to the U. S. Environmental Protection Agency throughout most of the preparation of this report. Since January 1982 he has been employed as an Environmental Meteorologist with NUS Corporation in Gaithersburg, Maryland.

PREFACE

Within the Office of Environmental Processes and Effects Research, the Environmental Sciences Research Laboratory conducts a research program in the physical sciences to detect, define, and quantify the effects of air pollution on urban, regional, and global atmospheres and the subsequent impact on water quality and land use. This includes research and development programs designed to quantitate the relationships between emissions of pollutants from all types of sources, air quality, and atmospheric effects.

The Meteorology and Assessment Division conducts research programs in environmental meteorology to describe the roles and interrelationships of atmospheric processes and airborne pollutants in effective air, water, and land resource management. One area of research within the Meteorology and Assessment Division is development, evaluation, validation, and application of models for air quality simulation, photochemistry, and meteorology. The models must be capable of describing air quality and atmospheric processes affecting the disposition of airborne pollutants, on scales ranging from local to global. Within the Division, the Environmental Operations Branch adapts and evaluates new and existing meteorological dispersion models and statistical technique models, tailors effective models for recurring user application, and makes these models available through EPA's computer system and UNAMAP.

Work described in this report explored the use of several alternatives to the standard use of a Gaussian-type air quality dispersion model and evaluated these methods with one-year data bases for two TVA power plants.

ABSTRACT

In this study, a routinely applied U. S. Environmental Protection Agency atmospheric dispersion model, MPTER, was used to develop and evaluate alternative modeling techniques. These modeling techniques incorporated into this model allowed for more detailed source data, onsite meteorological data, and several dispersion methodologies to be used. These alternative techniques were evaluated with hourly SO₂ concentrations measured at fixed receptors around coal-fired power plants near Paradise, Kentucky, during 1976 and near Johnsonville, Tennessee, during 1977. The data available for model input included the following:

- (1) hourly SO₂ emission rates and stack operating parameters,
- (2) hourly onsite wind data including measurements of sigma-theta and sigma-phi at the Johnsonville plant, and
- (3) hourly meteorology data from nearby National Weather Service stations.

The study also included a literature review of modeling techniques that can be incorporated into the MPTER model, an examination of previous case studies involving model evaluations, and an overview of validation procedures that have been recommended for evaluating air quality simulation models.

Seven alternative modeling techniques were developed for the Paradise plant, and 11 alternative techniques were developed for the Johnsonville plant. The Paradise alternatives included options in the following categories: source terms -- hourly and full load emission averages, meteorology -- routine airport data and onsite wind data, and dispersion -- Pasquill-Gifford parameters, Pasquill-Gifford parameters with buoyancy-induced dispersion, and Briggs rural interpolation formulae. The Johnsonville alternatives included options in the following categories: source terms -- daily emission averages, meteorology -- airport data with calm wind periods eliminated, and dispersion -- Pasquill's recommendations for including sigma-theta measurements to estimate sigma-y and adaptations of approaches by Draxler and Cramer to relate sigma-theta and sigma phi measurements to sigma-y and sigma-z, respectively.

The results of this study were used to assess the performance of the alternative techniques in estimating short-term peak SO₂ concentrations, especially those related to the National Ambient Air Quality Standards (NAAQS). The evaluation was accomplished mainly by comparing the peak predictions of the model results to the peak observations for each receptor. This type of unpaired comparison was necessary since wind direction errors causes uncertainty in determining the plume centerline position and hence assures low correlations between paired hourly observed and modeled concentrations.

A significant finding of the evaluation was that the more sophisticated models did not appreciably "outperform" the routinely applied models. The specification of source terms was an important consideration; but for Paradise,

the use of hourly average source terms resulted in underpredictions by about a factor of two. The use of the second category of modeling options, meteorology, resulted in small differences in model performance. In some comparisons, the models using airport meteorological data performed as well as the models using onsite wind data. The third category of modeling options, dispersion, included a rather large list of alternatives. With the Pasquill-Gifford and Briggs dispersion schemes, small differences in model performance were observed. More substantial differences occurred with models using onsite turbulence measurements. The model using Pasquill's recommendations tended to overpredict peak concentrations. The models based on Draxler's and Cramer's approaches using onsite turbulence yielded mixed results perhaps in part because the lateral standard deviation of wind direction available was the one-hour average of five-minute values (rather than a one-hour value) thus eliminating the longer period fluctuations that are of importance in estimating one-hour concentrations in addition to the shorter period fluctuations. Additional research is recommended to improve the application of onsite turbulence measurements and to provide more accurate estimates of plume trajectories for input to atmospheric dispersion models.

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Lastly, my appreciation is extended to my wife, Beth, for her many hours of sacrifice and words of encouragement.

SECTION 1

INTRODUCTION

BACKGROUND

Since World War I, attempts have been made to estimate the dispersion of air pollution sources. Sutton (1947) presented theories and equations of smoke dispersion based on his work with the British Chemical Defense Establishment in Porton, England, site of the first intensive dispersion experiment. Sutton's equations now serve as the basis for quantifying the impact of pollution sources.

In the United States, the first significant advances in air pollution modeling began when Congress passed Public Law 159 in 1955. This law called for the development of forecasting techniques and models in predicting air pollution levels. Other advances in air quality modeling resulted from the growth and subsequent regulation of the nuclear power industry. The United States Weather Bureau (1955) and Slade (1968) described techniques for estimating the dispersive processes associated with nuclear accidents and cooling tower emissions.

An additional impetus for air quality began with passage of the 1970 Clean Air Act (CAA). With the CAA, Congress created the U.S. Environmental Protection Agency (EPA), which was given the task of developing air quality models to ensure that various types of sources adhere to National Ambient Air Quality Standards (NAAQS).

OBJECTIVES

Despite the economic and environmental importance placed on air quality modeling, the predictions from dispersion models are often no better than within a factor of two of the observations (Hanna et al., 1977). Recognizing the limitations of these models, the EPA and the American Meteorological Society (AMS) are initiating steps to improve current modeling practices (Fox, 1981). The general consensus of the EPA and the AMS seems to be that more validations of air quality simulation models are needed to improve existing models and to guide the development of future models.

In this study, a point-source dispersion model designed for estimating the short-term sulfur dioxide concentrations around large smoke stacks was examined. Alternative modeling techniques were developed from this routinely applied Gaussian dispersion model and included different approaches for emissions, meteorology, and dispersion. This study seeks to evaluate a series of Gaussian plume dispersion models using data collected from two coal-fired power plants.

Specifically, the objectives of this research are as follows:

- 1) To modify a routinely applied Gaussian plume dispersion model and to evaluate alternatives that incorporate more realistic and/or more detailed information on meteorology, dispersion, and emissions;

- 2) To evaluate the benchmark model and the alternatives by using a year of data from two coal-fired power plants, including onsite meteorological measurements, a reasonably comprehensive SO_2 emissions inventory, and hourly SO_2 measurements collected from eleven to twelve receptor locations;
- 3) To assess the performance of the alternative models through statistical tests for peak concentrations and meteorological stratifications; and,
- 4) To isolate deficiencies in current modeling practices, determine if any of the alternatives offer improvements to predictions, and suggest how future calculations of point sources might be improved.

SECTION 2

SITE CHARACTERISTICS AND DATA ACQUISITION

The Tennessee Valley Authority (TVA) operates 12 coal-fired power plants that provide electricity to consumers in the Ohio River Valley. Since the 1950s, TVA has collected meteorological, SO_2 concentrations, and emissions data from these coal-fired power plants (Carpenter *et al.*, 1971). Data collected at the Paradise, Kentucky, power plant during 1976 and the Johnsonville, Tennessee, power plant during 1977, were used in this study. These plants were chosen for the evaluation of Gaussian plume dispersion models for the following reasons:

- 1) low background concentrations of SO_2 ;
- 2) absence of extreme topographical influences (both sites are characterized by rolling hills);
- 3) availability of two years of hourly onsite meteorology and SO_2 measurements; and
- 4) availability of data to derive hourly SO_2 emission rates and operating characteristics for each stack.

The data from these two power plants and from two National Weather Service (NWS) stations were used as model inputs. The locations of the two power plants, and the Evansville, Indiana (EVV), and the Nashville, Tennessee (BNA), NWS stations are shown in Figure 1.

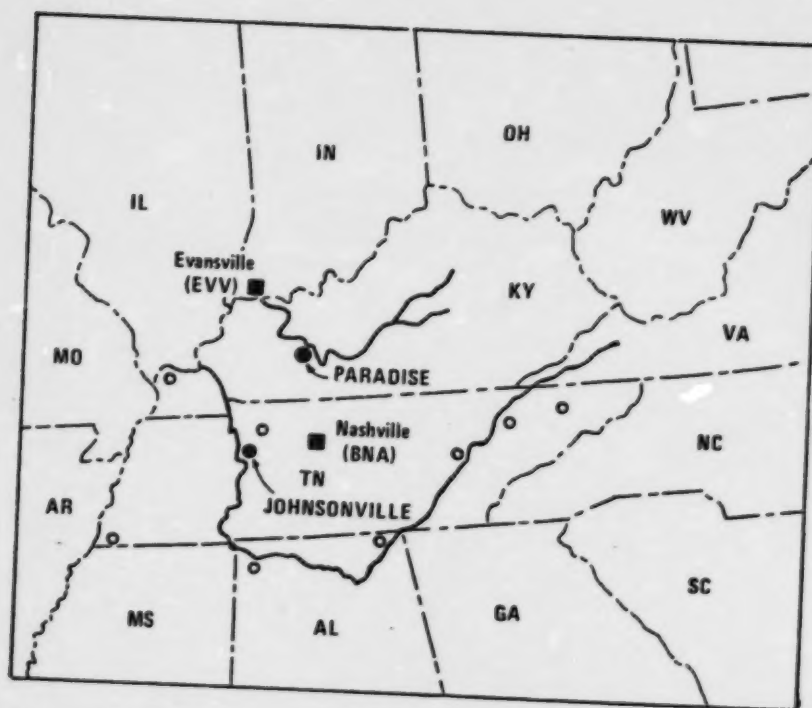


Figure 1. TVA coal-fired power plants (solid circles) and NWS stations (solid squares) used in the study.

JOHNSONVILLE

Construction of the ten turbines at the Johnsonville plant began in 1949 and was completed in 1959. The plant now has a generating capacity of 1.5 million kW. Eight stacks ranging in height from 82 m to 122 m are located at Johnsonville. The characteristics of these stacks are listed in Table 1. Hourly averages of SO_2 emission rates, stack gas temperatures, and stack gas exit velocities were estimated from daily coal consumption values and hourly power generation data. The procedures used to develop the stack parameters are explained in Appendix A. The variation in daily average SO_2 emissions derived for the Johnsonville site is depicted in Figure 2, and the diurnal change in the mean emission rate is shown in Figure 3. It should be noted from Figure 3 that the minimum mean hourly value at 4 a.m. was only 78 percent of the maximum mean hourly value computed at 8 p.m.

Onsite meteorological measurements were made from a 110 meter tower located 0.6 km south of the plant. Figure 4 shows the location of the plant, the meteorological tower, and the 11 SO_2 monitoring sites. The azimuth, distance, and the relative height above stack base of each receptor are listed in Table 2.

Phillips SO_2 monitors were used to measure SO_2 concentrations at the 11 sites. The technical specifications for the monitors are given in Table 3. At each monitoring site, samples were taken every minute, and the data were telemetered to a central data logging computer. Hourly averages of the SO_2 concentrations were recorded on magnetic tape.

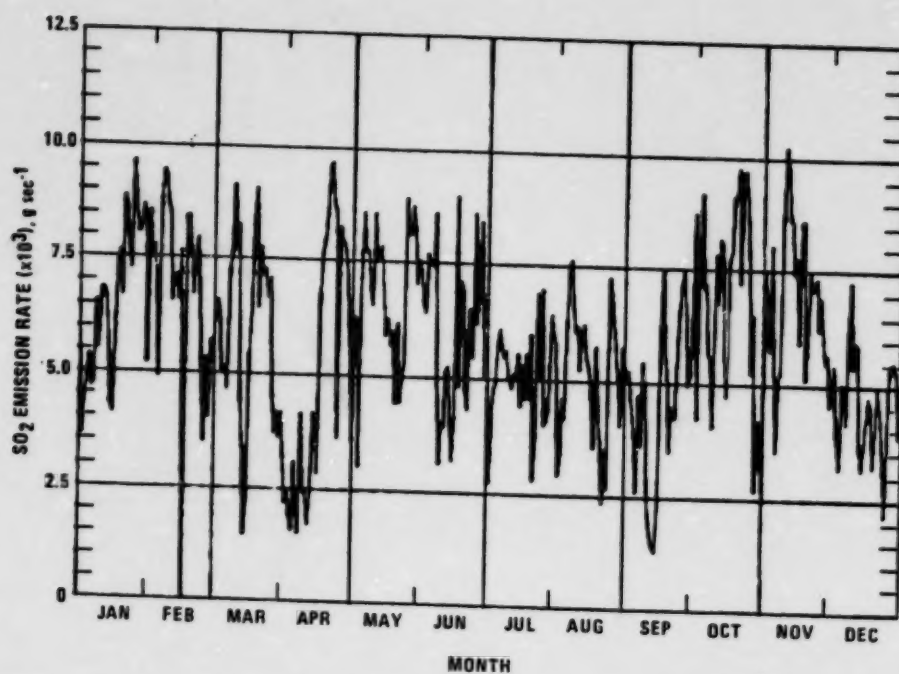


Figure 2. Average daily SO_2 emission rates for the Johnsonville, TN, power plant during 1977.

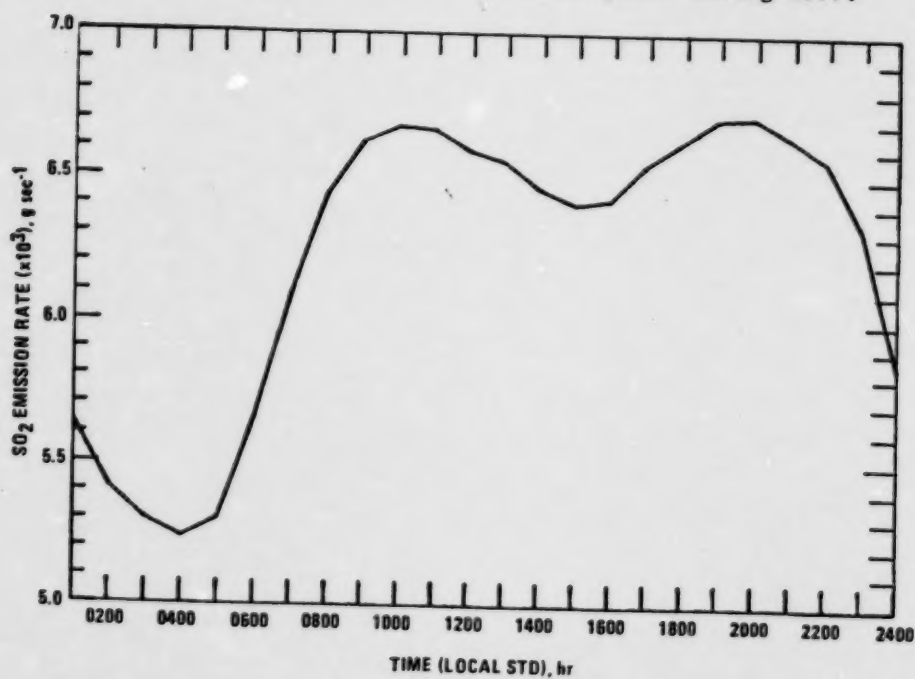


Figure 3. Diurnal variation of mean hourly SO_2 emission rates for the Johnsonville, TN, power plant during 1977.

TABLE 2. SITE CHARACTERISTICS AND DATA ACQUISITION OF THE JOHNSONVILLE SO₂ MONITORS DURING 1977.

Receptor number	Azimuth (degrees)	Distance (km)	Elevation above plant grade (m)	Percentage of missing SO ₂ data (n=8760 hrs)
1	41.7	4.57	-1.5	0.7
2	338.9	4.14	-1.5	0.4
3	134	3.33	25.9	0.7
4	268	5.31	13.7	11.2
5	6.2	6.55	47.2	0.7
6	36	3.27	42.7	0.6
7	61.5	3.70	59.4	4.0
8	94.5	5.15	24.4	89.3
9	156.2	5.71	1.5	1.6
10	232.5	8.66	10.7	0.9
11	296.2	5.07	21.3	0.4

TABLE 3. TECHNICAL SPECIFICATIONS OF THE PHILLIPS SO₂ MONITORS USED AT PARADISE AND JOHNSONVILLE

ITEM	DESCRIPTION
Design	Consists of two portable glass fiber reinforced polyester boxes which can stand on the ground or hang on the wall; one box contains the chemical section, where the measuring cell and calibration source are housed, and the other contains the electronics, pump, and telemetering system.
Measuring principle	Continuous coulometric titration with bromine.
Reproducibility	Better than 2% of the measuring signal.
Accuracy	Determined by accuracy of the SO ₂ source.
Accuracy of SO ₂ source	Within 15% of rated value over the first 3 months of delivery; better accuracy can be obtained by calibrating the SO ₂ source every 3 months against a weighted permeation source of by the West and Gaeke method.
Detection limit	Smaller than 10 $\mu\text{g}/\text{m}^3$ (4 ppb).
Size of zero current	Between 90 and 300 $\mu\text{g}/\text{m}^3$.
Drift of the zero signal	Smaller than 25 $\mu\text{g}/\text{m}^3$ per day, noncumulative at constant temperature.
Span drift	Less than 2% per day, noncumulative.
Response time	About 1.5 min (63% of final value); about 3 min (95% of final value).
Ambient temperature influence	Zero current variation per 10°C is less than a measuring signal corresponding to 25 $\mu\text{g}/\text{m}^3$ SO ₂ between 0 and 30°C; operation at lower or higher ambient temperatures is possible with extra provisions or some loss of accuracy.

TABLE 3. (continued)

ITEM	DESCRIPTION
Influence of humidity	Negligible.
Influence of mains variation	Ten percent mains voltage variation or frequency variation between 47 and 63 Hz has a negligible effect.
Output signal (before telemetry)	Zero to 20 mA, into 0 to 300 ohms for transmission, 100 mV for recorder.
Automatic calibration	Zero current and span can be remotely checked by means of a built-in zero filter and SO ₂ source; calibration can also be controlled by a plug-in clock module or manually; recommended program for automatic calibration is 30 min zero current check, 30 min calibration, and 11 hours of measuring.
Safety	In the chemical box, the highest voltage present is 36V.
Maintenance	Three months continuous operation without need for service or maintenance.
Power supply	110, 125, 145, 220, 235, or 250 V; 47 to 63 Hz; and 125 to 150 VA.
Weight	Complete, 65 kg.

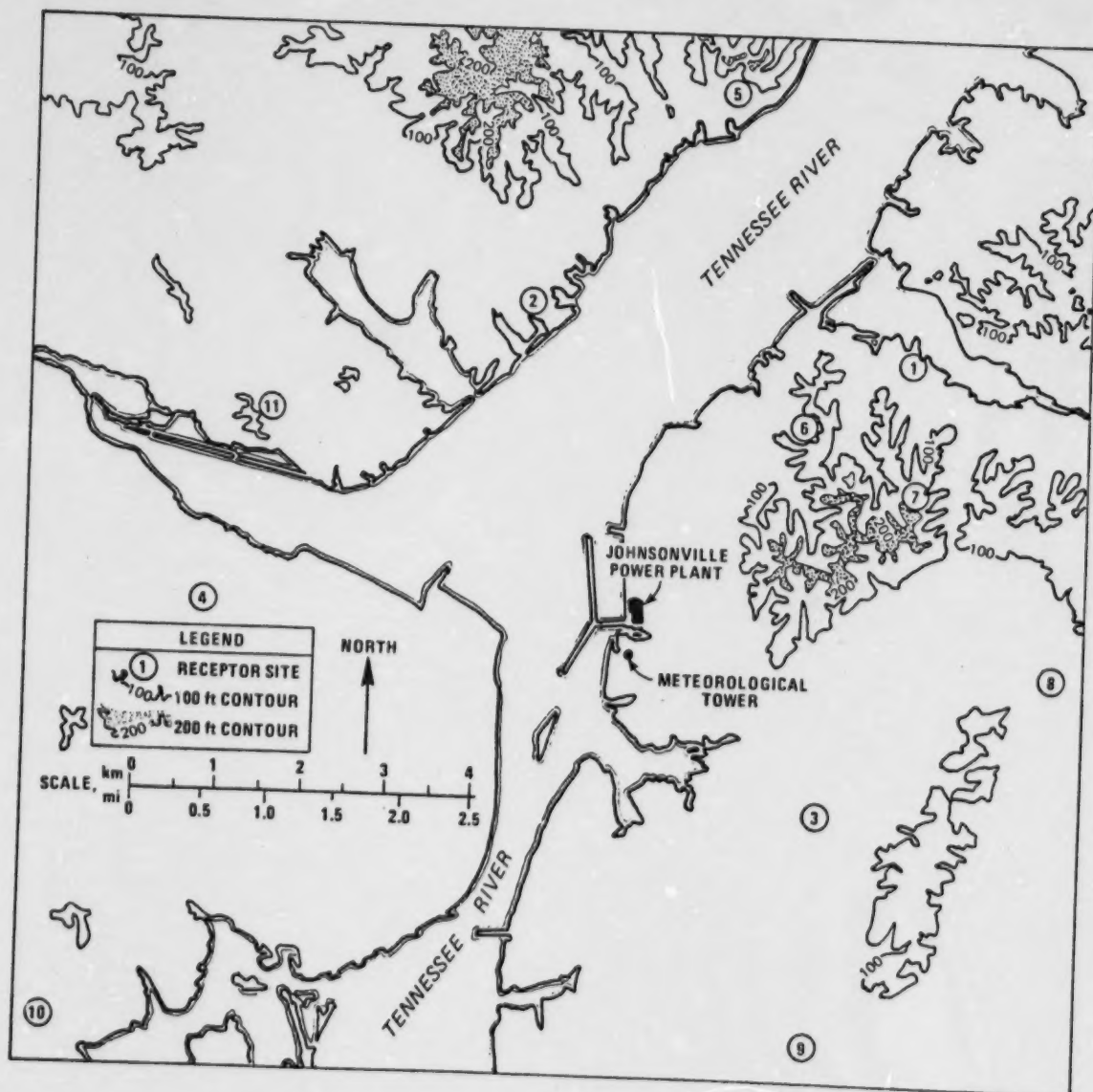


Figure 4. Johnsonville, TN, power plant site.

TVA personnel serviced the monitors at least once a week. In addition, technicians maintained around-the-clock surveillance at the central computing site to screen faulty data and to respond to equipment failures. This surveillance was part of a supplementary control program to reduce SO_2 emissions during critical meteorological periods (described by Leavitt *et al.*, 1971). The monitoring equipment were calibrated every 45 days to an accuracy of two percent. Automatic zero-level and calibration checks were also conducted daily at each monitoring site.

Onsite meteorological measurements were made at three levels, 1 m, 10 m, and 110 m. The technical specifications of the meteorological instruments are given in Table 4. The bivanes were located on booms that were oriented to the southwest in the direction of the prevailing winds. Wind speed, wind direction, and ambient air temperature were sampled every two seconds. The measured values were then telemetered to the central data logging computer, and hourly values were recorded on magnetic tape.

Standard deviations of the horizontal (σ_θ) and vertical (σ_ϕ) wind direction fluctuations were incorporated into the modeling analysis. The standard deviations were computed for each five-minute period by using the measurements made every two seconds. The five-minute values were then averaged for each hour. The hourly averaged σ_θ values from measurements made at the 10-meter and 110-meter levels, and hourly averaged σ_ϕ values from measurements made from the 110-meter level were stored on magnetic tape.

TABLE 4. SENSOR SPECIFICATIONS OF THE METEOROLOGICAL INSTRUMENTS USED AT THE JOHNSONVILLE POWER PLANT DURING 1977

SENSOR	LEVELS (m)	DESCRIPTION
Wind speed	10, 110	Climet Instruments, Inc., Model 011-1: starting threshold, 0.3 ms^{-1} ; calibrating range, $0.3 - 40.2 \text{ ms}^{-1}$; operating range, $0 - 49 \text{ ms}^{-1}$; data recording range, $0 - 44.7 \text{ ms}^{-1}$; accuracy, $\pm 1\%$ or 0.07 ms^{-1} whichever is greater at $0.3 - 40.2 \text{ ms}^{-1}$.
Wind direction	10, 110*	Climet Instruments, Inc., Model 012-10: calibrated range, (electrical) $0 - 540^\circ$ (mechanical) $0 - 360^\circ$; data recording range, $0 - 540^\circ$ ($0-4.8\text{V}$); linearity, $\pm 0.5\%$; accuracy, $\pm 3^\circ$.
Ambient air temperature	1, 10, 110	Climet Instruments, Inc., Model 016-1: data recording range, -23.3 to 37.7°C ; RTD accuracy, $\pm 0.03^\circ$; aspirated shield

* bivan used at 110 m

Excluding the computations for σ_θ and σ_ϕ , only 4.6 percent of the hourly meteorological data collected at Johnsonville during 1977 were missing. Including the σ_θ computations, 8.2 percent of the data were missing; including the σ_ϕ computations, 22.4 percent of the data were missing.

PARADISE

With the completion of third unit in 1970, the Paradise power plant became the largest electrical generating facility east of the Mississippi River. The plant has a total generating capacity of 2.6 million kW and can burn 2,100 tons of coal per day. Three stacks disperse the gaseous effluents from the Paradise site: two stacks 183 m high and one stack 244 m high. The characteristics of each stack are noted in Table 5. Similar to Johnsonville, hourly averages of the SO_2 emissions, exit velocities, and stack gas temperatures were approximated from the data available for daily coal consumption and hourly power generation. The methodology for this procedure is outlined in Appendix A. The diurnal variation in mean SO_2 emissions for Paradise is plotted in Figure 5. The minimum mean computed at 2 p.m. is 96.8 percent of the maximum mean emission computed at 10 p.m. The day-to-day variation in the SO_2 emissions from Paradise during 1976 is plotted in Figure 6.

Meteorological measurements were taken from a 110-meter tower located 1.5 km west of the Paradise plant. Figure 7 shows the location of the plant, the meteorological tower, and the 12 SO_2 monitoring sites. The monitors were located at distances ranging from 2.9 km to

TABLE 5. STACK CHARACTERISTICS AT THE PARADISE TVA POWER PLANT

Parameter (units)	Stack number		
	#1	#2	#3
Height (meters)	182.9	182.9	243.8
Diameter (meters)	7.92	7.92	8.17
Stack gas temperature (K)			
@100% capacity	416.5	416.5	416.5
@75% capacity	412.6	412.6	413.7
@50% capacity	410.4	410.4	405.9
Stack exit velocity (m/s)			
@100% capacity	17.13	17.13	26.12
@75% capacity	13.23	13.23	18.78
@50% capacity	9.20	9.20	14.20
Generating capacity (MW)	704	704	1150.2

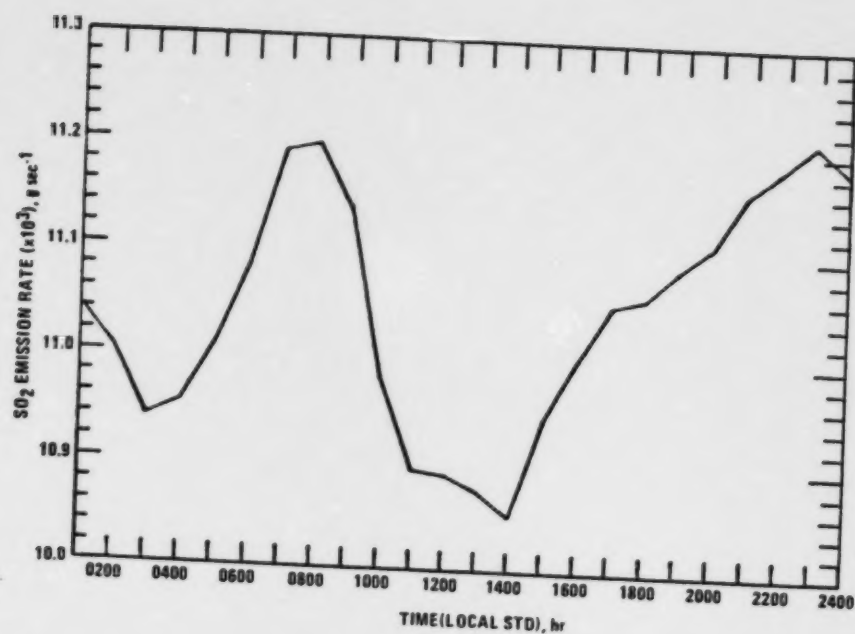


Figure 5. Diurnal variation of mean hourly SO₂ emission rates for the Paradise, KY, power plant during 1976.

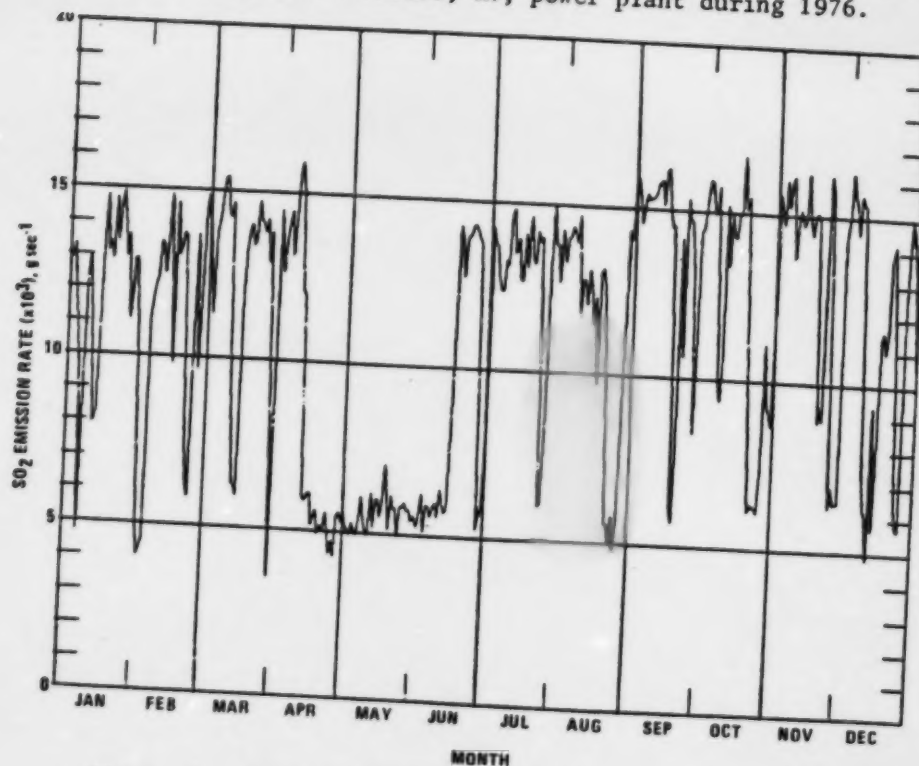


Figure 6. Average daily SO₂ emission rates for the Paradise, KY, power plant during 1976.

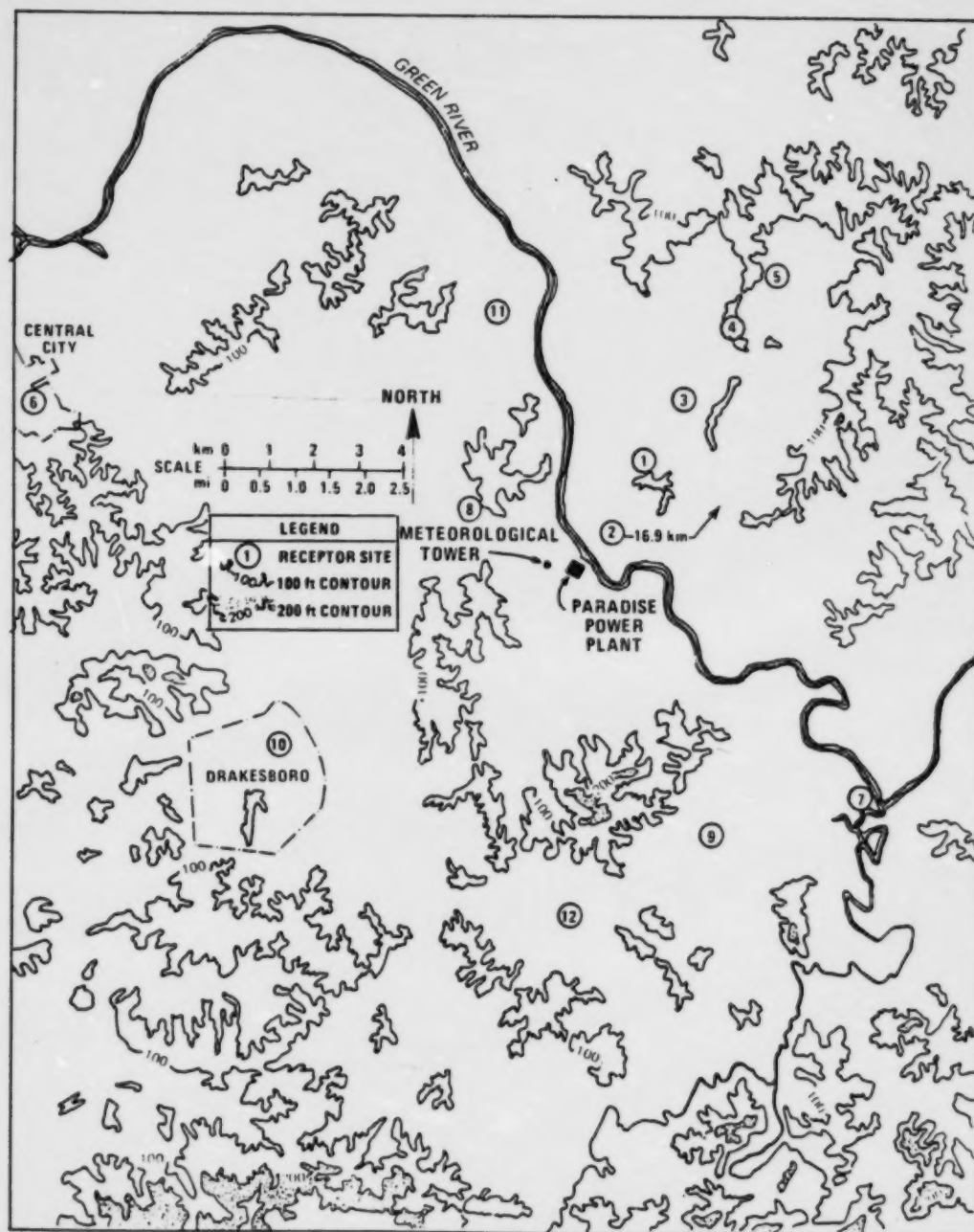


Figure 7. Paradise, KY, power plant site.

16.9 km from stack #1. The azimuth, distance from the plant, relative height above stack base, and percentage of missing data collected during 1976 for each monitor are presented in Table 6. Because the area around the plant is typified by rolling hills having a relief generally less than 25 percent of the stack heights, it appeared that plume transport and dispersal were not significantly influenced by topography.

Phillips SO₂ monitors, identical to those used at Johnsonville, were used at Paradise. The data acquisition procedures, and the maintenance and calibration schedules were also the same as those used at Johnsonville.

The specifications for the meteorological instruments used at Paradise were also the same as those followed at Johnsonville and are given in Table 4. The onsite meteorological measurements were unfortunately less comprehensive than those collected at Johnsonville. Approximately 96 percent of the data collected onsite were available for 1976. The meteorological parameters included hourly averages of wind speed, wind direction, and ambient air temperature. The data acquisition procedures and the averaging procedures used with the Paradise meteorological data were the same as those used at Johnsonville.

TABLE 6. SITE CHARACTERISTICS AND DATA ACQUISITION OF THE PARADISE SO₂ MONITORS DURING 1976

Receptor number	Azimuth (degrees)	Distance (km)	Height above plant grade (m)	Percentage of missing SO ₂ data (n=8784 hrs)
1	31	2.9	-1	62.1
2	47	16.9	24	61.4
3	31	4.67	21	3.7
4	31	6.76	36	61.6
5	32	8.37	15	61.6
6	284	12.7	12	1.8
7	126	8.53	-7	1.4
8	301	3.38	16	2.8
9	150	7.0	15	1.8
10	238	7.66	22	0.3
11	342	6.05	2	0.6
12	178.5	7.90	10	0.6

SECTION 3

LITERATURE REVIEW

TECHNICAL BACKGROUND

Present-day Gaussian plume dispersion models are based on the theory of heat diffusion extended by Albert Fick in the mid 1800s. Sutton (1947a, 1947b) adapted Fick's theory into rather simple mathematical equations for estimating the dispersal of gaseous effluents. The derivations of the Gaussian plume dispersion equations are described in Sutton's (1953) classic text Micrometeorology.

The approximate Gaussian spreading of a plume was established with measurements taken from the Porton Field Study in 1923 (Pasquill, 1974). The Gaussian distribution, shown in Figure 8, is often estimated with empirical formulations of the horizontal dispersion coefficient, σ_y , and the vertical dispersion coefficient, σ_z . Incorporating the experimental results from the Porton Field Study and the 1957 Prairie Grass Field Study, Pasquill (1961) tentatively offered a scheme for estimating the dispersion of a surface release, within one kilometer, in terms of broad stability classes. Gifford (1960) adapted Pasquill's work and derived solutions for σ_y and σ_z . The graphs of σ_y and σ_z as functions of distance for each Pasquill stability class are shown in Figure 9. The dashed lines in Figure 9 indicate that extrapolations of the original tracer data were used to develop the curves.

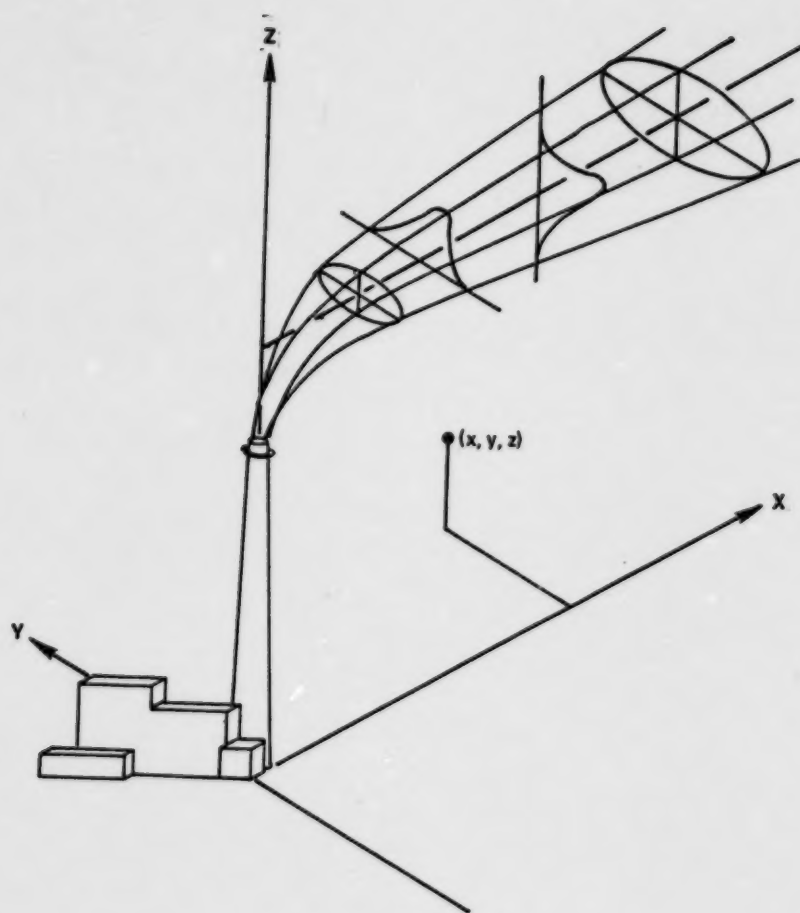


Figure 8. Coordinate system showing horizontal and vertical Gaussian distributions.

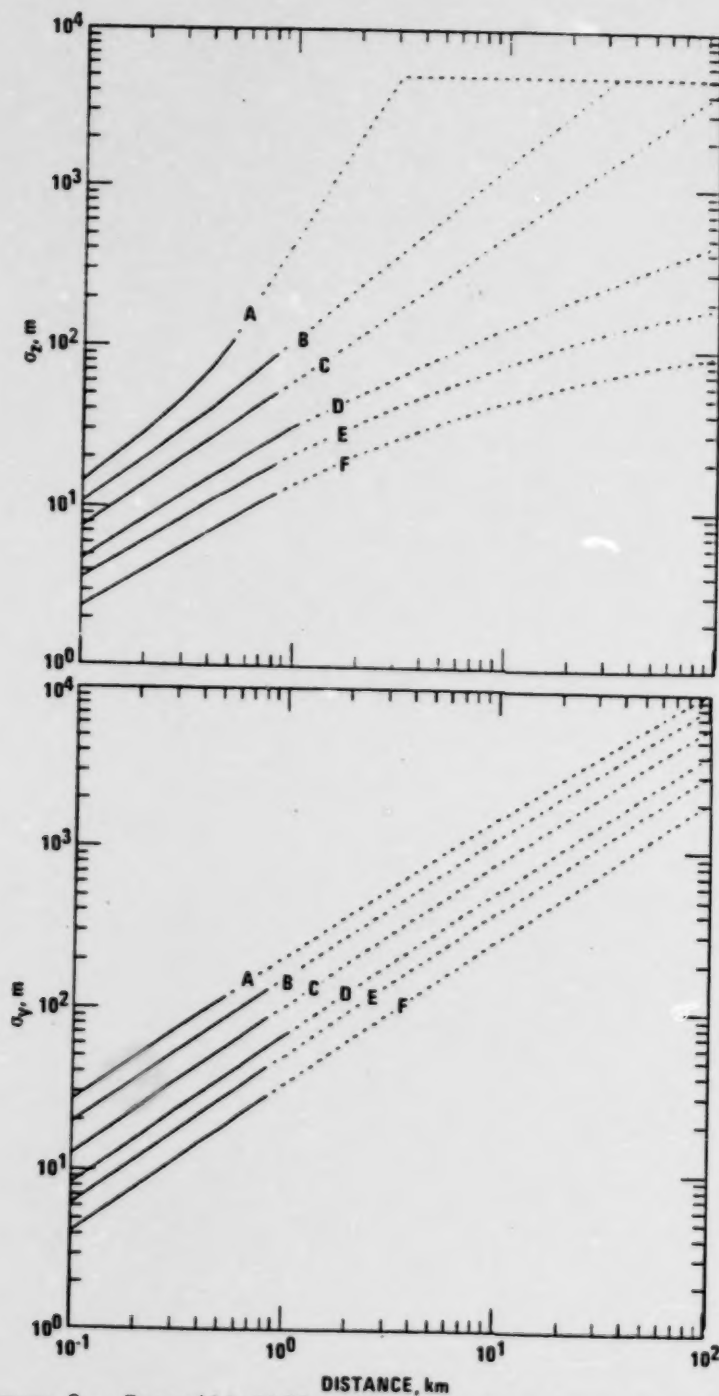


Figure 9. Pasquill-Gifford curves of horizontal (σ_y) and vertical (σ_z) dispersion as a function of distance and stability class. (Curves generated from a computer algorithm of Turner, 1981. Dashed lines represent extrapolations of field data.)

Turner (1964) then developed objective criteria for estimating Pasquill stability classes in terms of routine measurements of wind speed, cloud cover and ceiling height, and solar insolation. Turner's method and Pasquill-Gifford dispersion coefficients (also known as PG curves) now form the dispersion algorithms of most Gaussian plume dispersion models.

Alternative Dispersion Coefficients

The EPA Gaussian plume dispersion model used in this study incorporates the Pasquill-Gifford (PG) dispersion coefficients. Other dispersion coefficient schemes abound in the literature, and excellent summaries of these schemes are given by Slade (1968) and Gifford (1976). The schemes appropriate to the development of the alternative models are discussed below.

A noteworthy scheme was developed for elevated releases from tracer studies conducted at Brookhaven National Laboratory during the early 1960s. The development of the Brookhaven curves is outlined by Singer and Smith (1953) and by Singer et al. (1966). Smith (1968) edited a guide for the American Society of Mechanical Engineers (ASME) and presented the Brookhaven curves as graphs (shown in Figure 10) of σ_y and σ_z as functions of downwind distance, x . Applying the Brookhaven curves to the Johnsonville and Paradise sites was a problem because the curves are based upon site-specific gustiness criteria developed for Brookhaven (Gifford, 1976), and the necessary data for applying the curves to Johnsonville and Paradise were not available. Thus, the Brookhaven curves were not evaluated in this study.

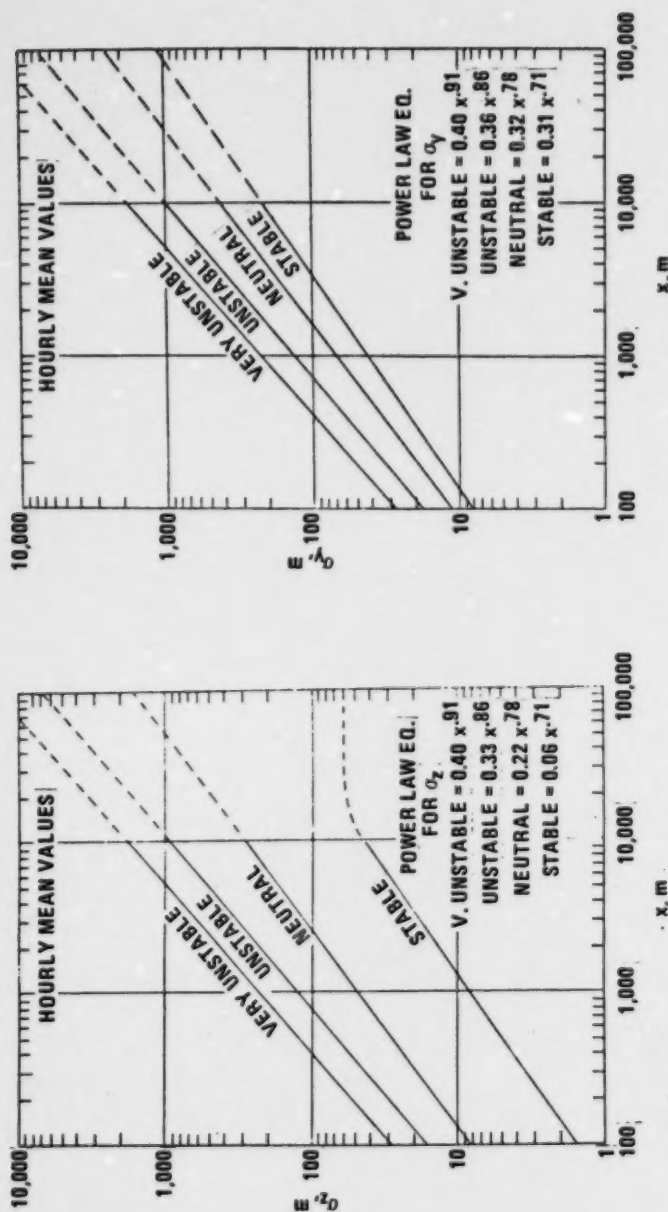


Figure 10. Brookhaven dispersion curves from Smith (1968).

Briggs' scheme for estimating rural dispersion coefficients incorporated the experimental results from both the Brookhaven and the PG curves. Gifford (1976) listed Briggs' interpolation formulae for estimating the dispersion of elevated releases by using Pasquill stability classifications. As shown in Figure 11, the major difference between the PG curves and the Briggs curves occurs with σ_z for stability class A. After a distance of 100m, the Briggs curve during A-stability increases less rapidly with distance than the PG curve. A FORTRAN algorithm incorporating the Briggs interpolation formula was developed for this study and is presented in Appendix B.

The use of onsite turbulence measurements to directly estimate dispersion has been encouraged by Pasquill (1961, 1974, and 1976) and by the American Meteorological Society (AMS) (Hanna *et al.*, 1977). Three approaches based on studies by Pasquill (1976), Draxler (1976), and Cramer (1976) were used in this study with the turbulence data collected at the Johnsonville plant.

In proposing changes to the dispersion curves of Turner (1970), Pasquill (1976) recommended that measurements of horizontal wind direction fluctuations be used to estimate σ_y and that the PG curves, with minor adjustments, be used to estimate σ_z . Pasquill related σ_y to the standard deviation of wind direction fluctuations, σ_θ , as follows:

$$\sigma_y = \sigma_\theta \times f(x)$$

where x is the downwind distance (in meters) and $f(x)$ is a function of downwind distance, with values for $f(x)$ prescribed by Pasquill. An approximation to $f(x)$ is given by the following:

$$f(x) = 1/[1 + (x/2500)^{1/2}]$$

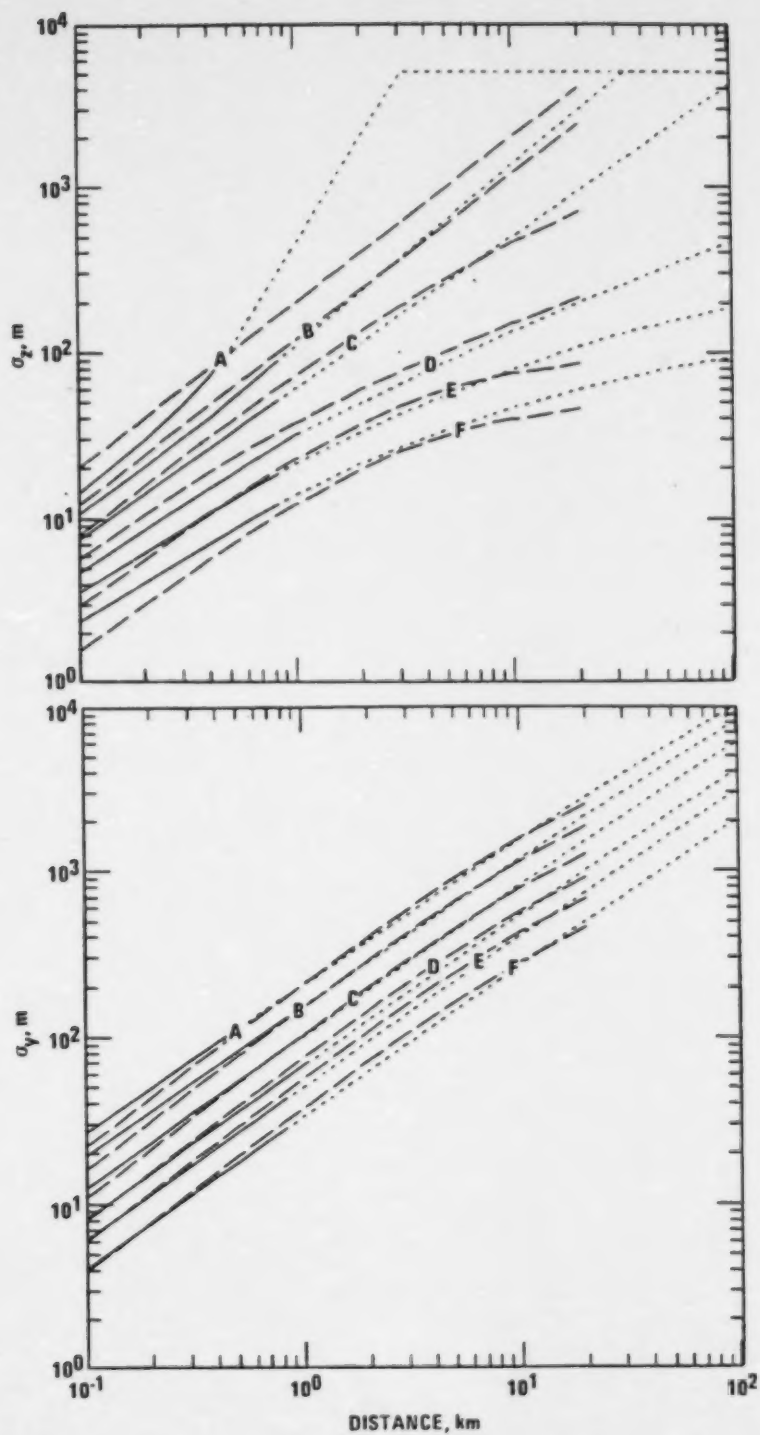


Figure 11. Comparison of Briggs interpolation formulae as indicated by long-dashed lines and the PG curves as a function of distance and stability class.

Adhering basically to Taylor's (1921) statistical theory, σ_y thus increases linearly for short travel times but approaches a growth rate of $x^{1/2}$ for longer travel times.

Because Pasquill believed that instruments were of insufficient quality to estimate vertical wind direction fluctuations, he recommended that the PG curves for σ_z be employed, with adjustments made for surface roughness, urban heating, effect of the mixing depth, and buoyancy-induced-dispersion. These recommendations, as abstracted from Pasquill (1976), are presented in Table 7.

A FORTRAN algorithm incorporating Pasquill's recommendations was written for this study and is listed in Appendix B. The following assumptions were made in applying the algorithm to the Johnsonville site:

- 1) No adjustment for surface roughness was made, because the roughness length characterizing the Johnsonville site was not significantly greater than that calculated for Prairie Grass (0.03 m).
- 2) No adjustment to account for urban heating effects was necessary.
- 3) The effects of buoyancy-induced-dispersion were added for σ_y and σ_z .

TABLE 7. SUMMARY OF RECOMMENDATIONS FOR INTERIM CHANGES IN THE WORKBOOK VALUES OF THE DISPERSION PARAMETERS σ_y and σ_z
(after Pasquill, 1976)

For crosswind spread σ_y , irrespective of the terrain roughness, release height and sampling duration up to about 1 hour, use the formula

$$\sigma_y/x = \sigma_y f(x), \sigma_y \text{ in radians}$$

with σ_y the best available estimate of the standard deviation of the wind direction fluctuation for the sampling time of interest and for the height at which u is specified, and with values of $f(x)$ as follows:

x (km)	0.1	0.2	0.4	1	2	4	10	>10
$f(x)$	0.8	0.7	0.65	0.6	0.5	0.4	0.33	$0.33(10/x)^{1/2}$

For $x \geq 20$ km add to the square of the σ_y as obtained above the quantity $0.03 \Delta \theta^2 x^2$ and take the square root to give the total σ_y , with $\Delta \theta$ the total change of mean wind direction over the depth of the plume.

For vertical spread σ_z , for any sampling time for a surface release, and say >10 min for an elevated release (see Section 2), use the existing Workbook curves with adjustment or constraint as follows:

- For terrain with z_0 different from 3 cm apply factors based on F. B. Smith's nomogram (Ref. 5 or Ref. 6, p 377)
- To allow for 'urban heating' adopt a stability category one-half category more unstable than than prescribed in the normal way in the Workbook
- For evaluating the concentration at the surface from a surface release, consider estimates of the effective mixed depth h' at the mid-time of sampling, recognizing especially its growth from very small values on stable nights, and then adopt either σ_z as given by the curves, or $0.8h'$, whichever is the smaller, for substitution in Eq (4).
- For buoyant plumes, increase the σ_z^2 obtained from the curves by adding $\Delta H^2/10$ where ΔH is the estimated plume rise.

To relate measurements of σ_θ and σ_ϕ to estimates of σ_y and σ_z , respectively, Draxler (1976) developed the following functions:

$$\sigma_y = \sigma_\theta \times f(t/T_i)$$

$$\sigma_z = \sigma_\phi \times f(t/T_i)$$

where x is the travel distance (in meters), t is the time for the plume to travel to x , and T_i is a constant that is proportional to the Lagrangian time scale or the diffusion time required for $f(t/T_i)$ to reduce from 1.0 to 0.5. Although Draxler presented functions for both surface and elevated releases, only the functions for an elevated release were examined with the Johnsonville turbulence data.

To estimate horizontal diffusion for all stability classes and vertical diffusion for unstable conditions, Draxler recommended the following equation:

$$f(t/T_i) = 1/\{1 + 0.90 (t/T_i)^{1/2}\}$$

where $T_i = 1,000$ s for horizontal diffusion, and $T_i = 500$ s for vertical diffusion during unstable conditions. To estimate the vertical diffusion during stable conditions, Draxler suggested the following function:

$$f(t/T_i) = 1/\{1 + 0.945 (t/T_i)^{0.806}\}$$

where $T_i = 100$ s. Draxler cautioned against using the equation above during stable conditions, as only limited data were available to develop the function. He also noted that the decoupling of the atmosphere during stable conditions could hamper the equation's usefulness.

A FORTRAN algorithm incorporating Draxler's equations was developed for this study and is listed in Appendix B. Preliminary testing of the algorithm showed that turbulence data collected at Johnsonville during stable conditions resulted in unrealistically high surface concentrations. As an interim measure for this study, σ_z values associated with ambient turbulence were set at to 0.1 m during the nighttime hours.

Drawing upon his experience in diffusion meteorology, Cramer (1976) also devised an empirical approach that related σ_y and σ_z to σ_θ and σ_ϕ , respectively. Although he presented equations that resembled Draxler's formulations, Cramer used the concept of a virtual distance to account for buoyancy-induced-dispersion and the nonlinear growth of σ_y . Bjorklund and Bowers (1979) noted that in Cramer's scheme that σ_y increases as a function of $x^{0.9}$. They argued further that wind shear effects probably cause σ_y to increase as a function of approximately $x^{0.9}$ instead of $x^{1/2}$, as suggested with Taylor's statistical theory. This seems to be a reasonable assumption, because Pasquill (1976) recommended that wind shear effects be incorporated into σ_y for downwind distances greater than 20 km.

Cramer's equations for σ_y and σ_z can be simplified to the following:

$$\sigma_y = 1.63 \sigma_\theta (x + x')^{0.9}$$

$$\sigma_z = \sigma_\phi (x + x_z)$$

where x is the downwind distance (in meters) and x' and x_z are empirically derived values that basically account for buoyancy-induced-dispersion. A FORTRAN algorithm incorporating Cramer's ideas was developed for this study and is presented in Appendix B.

MODEL EVALUATIONS

Much attention has been given to the technical basis for air pollution models, but the ultimate concern is just how well do the model estimates compare with actual measured concentrations. Numerous studies have been completed that examined such comparisons and are identified by a number of terms, including validation, evaluation, sensitivity analysis, verification, comparisons, calibration, and qualification. Two articles by Turner (1979) and Benarie (1980), in fact, include semantic discussions of these terms.

For this study, evaluation is taken to mean a comparison of model estimates with measurements. It also "implies that comparisons have been made with a variety of partitioning of the data so that the performance of the model can be determined for a variety of conditions, such as different meteorological conditions" (Turner, 1979). Validation, in this study, is defined as a rigorous study usually involving extensive field data to establish the accuracy of a model or a technique such as a dispersion coefficient scheme. The emphasis below is to survey previous model evaluations and to concentrate on those procedures that could be used in evaluating point source dispersion models.

Field Studies

Early model validation studies incorporated data collected from field studies, such as the Porton Field Study (Pasquill, 1961) and the Prairie Grass Field Study (Barad, 1958). These two studies were designed specifically to examine the Gaussian plume dispersion hypothesis and to establish methods for estimating plume dispersion.

In a rigorous tracer study like the Prairie Grass Field Study, a substance such as SF_6 , whose composition is well understood and whose release is carefully controlled, is emitted and subsequently sampled at a pre-selected array of receptors. These receptors are usually positioned in a sufficiently dense array to establish the position and horizontal spread of the plume. A sizeable amount of meteorological data usually complements the tracer measurements; in the Prairie Grass Field Study, state-of-the-art turbulence measurements were utilized. The experimental approach and data analysis procedures deployed during the Prairie Grass Field Study and later field experiments have been summarized by Slade (1968). Due to the expense involved, however, only a limited number of intensive field studies have been performed.

In a recent field study (Gogolak et al., 1981), the Savannah River Laboratory served as the site for an elevated release, long-term tracer study. The tracer Krypton-85 was emitted from a height of 62 m during 1976. Meteorological parameters, including σ_θ , were measured at release height. Tracer measurements were collected at six monitors located within ten kilometers of the release tower. Using the formulations suggested by Smith (1968), Gogolak et al. compared the ratios of the geometric mean of observed to predicted concentrations from the year of available data. While these ratios were within a factor of two, unusually high hourly predictions were noted under stable conditions, especially when $\sigma_\phi < 3^\circ$ and $u < 3$ m/s. These high predictions were attributed to problems in defining the plume trajectories.

Present knowledge of atmospheric dispersion processes is hampered by a lack of field data, particularly in complex situations. Two field studies were recently initiated that should provide information to help improve current modeling techniques. The first study known as the Small Hill Study (Holzworth, 1980) involved tracer releases around a 100 m hill in Idaho. The experimental portion of this study was completed in April 1981. Dispersion models designed for elevated terrain applications are presently undergoing development and evaluation by ERT, Inc. The second study, termed PMV (Plume Model Validation) (Bowne and Hilst, 1981), involved a tracer study at a relatively isolated coal-fired power plant in Illinois. Funded by the Electric Power Research Institute (EPRI), this study is attempting to evaluate the performance of Gaussian plume dispersion models.

Routine Analysis

Because of a lack of intensive field experiment data, researchers have relied upon routine monitoring data to investigate the performance of air quality simulation models. A comprehensive survey of the routine monitoring data available for model evaluations was conducted by Sklarew and Joncich (1979). The discussion presented below emphasizes only those procedures that were considered for analyzing model results from the Paradise and Johnsonville power plants.

In evaluating the performance of the widely applied single-source model, CRSTER (EPA, 1977), Mills has provided a voluminous account (Mills and Record, 1975; Mills and Stern, 1975; Mills and Stern, 1977; Mills, 1977) on the performance of the CRSTER model with data from three Ohio power plants and a power plant in Massachusetts.

In comparing observations to predictions, Mills relied extensively on cumulative frequency distributions of hourly, 3-hour, and 24-hour average concentrations. Mills noted little agreement between paired measured and modeled concentrations. According to Tikvart and Mears (1976), the CRSTER model was reasonably "validated" by Mills for estimating concentrations used in regulatory analysis. Mills' application of CRSTER does, however, raise some questionable points:

- 1) Monthly average sulfur values were used in computing hourly SO_2 emission rates.
- 2) Onsite meteorological data were lacking, and airport data from locations over greater than 50 km from the site were used.
- 3) The statistical analysis emphasized the peak unpaired concentrations, and only a marginal attempt was made to stratify the data by meteorological regimes.

In assessing Mills' analysis to the analysis for the Johnsonville and Paradise sites, several improvements were planned for incorporation into this study:

- 1) Weekly instead of monthly average sulfur values were used to develop hourly SO_2 emissions.
- 2) Comprehensive onsite meteorological data were available and were compared against nearby airport meteorological data.
- 3) The modeled and observed concentrations were stratified by stability, so that possible causal explanations of model performance could be hypothesized.

In a study of power plant in complex terrain, Ellis et al. (1980) applied 52 alternatives of the CRSTER model to a year of data.

The investigation of overall model performance lacked detailed information as to why the model alternatives either underpredicted or overpredicted peak concentrations. Nevertheless, the matrix approach of model alternatives used by Ellis is useful because it allows for an examination of a wide range of modeling techniques. This matrix approach was used to some extent in developing the alternative models for Paradise and Johnsonville.

In the first of two previous model evaluations involving the Paradise plant, Enviroplan (1976) examined model results and monitoring data collected during 1970. The data base consisted of hourly SO_2 emissions data, hourly averaged SO_2 measurements from 14 receptors, and onsite meteorological data. The CRSTER model was analyzed by using onsite wind measurements; stability class data from Evansville, Indiana (EVV); and mixing heights from Nashville, Tennessee (BNA). The evaluation focused primarily on the model's ability to predict peak 3-hour and 24-hour concentrations. The following conclusions were noted from the study:

- 1) Poor correlation between was computed between paired modeled and measured concentrations at all monitoring sites.
- 2) The ratios of measurements to predictions varied immensely, but there was a tendency for the model to overpredict.
- 3) Model overprediction was especially prevalent for the peak concentrations.

Although onsite wind measurements were used in the modeling, the wind directions were only read from the last 60 seconds of each hour and then randomized within a ten degree sector.

The second model evaluation performed with Paradise data involved a limited study by Klug (1975). Data for 1971 were used that included the following parameters: onsite wind and temperature measurements, hourly SO₂ measurements from eight receptors, and hourly SO₂ emission rates. Klug limited comparisons between modeled and measured concentrations to hours when the onsite wind vectors at 110 m were directed within a 45° sector directed towards each receptor. Stability classes were computed by using temperature lapse rates. Klug also improved correlation coefficients by altering the wind direction. His results showed that predicted annual concentrations were within a factor of two of observed annual concentrations. Altering the wind directions "improved" correlation coefficients from 0.15 to 0.40. As in other point source evaluations, large standard errors were computed between paired hourly values, thus indicating that the Gaussian plume dispersion model could not accurately predict hourly concentrations because of its sensitivity to wind direction. Klug also investigated a routine for accounting for surface roughness (F. Smith, 1972) but noted no significant improvements in model predictions.

Other articles on model evaluation, too numerous to review here, cover a wide variety of model types, averaging times, pollutant species, topographical considerations, monitor arrays, stack types, and meteorological data. The articles that were examined for this study are referenced in the bibliography.

VALIDATION PROCEDURES

The above survey has shown that many types of statistical tests are used to assess model performance. The lack of consistency used in applying these statistical tests has been a subject of concern in recent years. This section reviews many of the procedures that have been recommended for validating dispersion models.

Johnson (1972) was among the first to note the need for performance measures in model validation. He pragmatically demonstrated that the difficulty in testing model performance resulted from differences in the application of dispersion models, and variations in the quality of model input data. Johnson suggested that incorrect emissions data were probably the weakest link in model performance. He also stated that the validation of air quality models should be divided into a validation of individual modules; such as emissions, dispersion, transport, and chemical transformations.

Following a similar view as Johnson, Calder (1974) noted the differences between how decision makers view models and how scientists develop and apply these models. Calder noted that the decision maker demands a single extreme value (such as the second highest 24-hour average concentration) from a distribution of concentrations, whereas the modeler is more concerned with the model's overall ability to estimate median values and distributions. He thus recommended that decision makers and others who misapply models become aware of the limitations of air quality simulation models. To further emphasize his

argument, Calder quoted the following statement by Scorer (1970):

"There are no universal formulae which can be used to describe what will happen to pollution emitted into the air, and this needs to be said because formulae have been so misused in the past by people who have been secretly frightened of realities and have dispensed according to the prescription of the most fashionable wizard."

Calder mentioned that many models with only slight variations were being applied. He emphasized, like Johnson, that the individual modules in each model should first be validated because so-called validations of the entire model were but crude calibrations of predicted to observed concentrations. The underlying theme in Calder's treatise is that little statistical significance can be placed on a model that is being used to predict only extremes of a frequency distribution.

Beginning with Brier (1975), actual statistical measures were presented for performing model validations. Although Brier's work is basically a pure statistical discussion, the following general steps were presented for performing a model validation:

- 1) Complete a sensitivity analysis of the model.
- 2) Calculate mean square errors of the residuals (differences between predicted and observed concentrations).
- 3) Complete a regression analysis of predicted and observed concentrations.
- 4) Examine the frequency distributions of predicted and observed concentrations.
- 5) Examine the overall bias of the model.

Like Calder and Johnson, Brier emphasized that a good validation should at least provide clues on what part or module of the model is responsible for the errors.

During the 1970s, various statistical tests were used in model evaluation studies. Bornstein and Anderson (1979) reviewed many of these studies and recommended a general approach to model validation by suggesting a mixture of qualitative and quantitative measures. Reiterating earlier researchers, Bornstein and Anderson pointed out that the primary source of model error is the quality of the input data. They recommended the following characteristics for a validation:

- 1) Examine the entire range of conditions (all data).
- 2) Look at specific conditions.
- 3) Examine different averaging periods.

Bornstein and Anderson cautioned that specific measures be restricted to individual sites to avoid averaging the overpredictions and underpredictions between different sites. The statistics they recommended included mean values, standard deviations, standard errors of the estimates, and correlation coefficients. They also recommended that isopleth plots, scatter plots, and cumulative frequency distributions be used for model validations.

Recognizing the need for having a quantitative model evaluation package, Bencala and Seinfeld (1979) introduced a FORTRAN algorithm called AQMAAP. They reviewed a number of statistical techniques and included the statistics shown in Table 8 into AQMAAP. Although Bencala and Seinfeld offer a number of useful statistical tests, their emphasis is on the evaluation of urban/photochemical-type models.

TABLE 8. METHODS FOR ASSESSING MODEL PERFORMANCE INCLUDED IN AQMAAP
(after Bencala and Seinfeld, 1979)

Analysis of Residuals

Mean error

RMS error centered at mean error

Absolute error band

Percentage error band

Residual histogram

Residual vs. time plot

Residual vs. observed magnitude plot

Residual vs. location plot

Analysis of Trends

Correlation trends

Regression analysis

Analysis of Indices of Air Quality

Magnitude and time of concentration peaks

Location of concentration hot spots

Exposure

Geometric parameters of highest values

Frequency distribution

Rao and Visalli (1981) recognized that the reliability and accuracy of air quality models were not well-documented due to a lack of field data and well-defined performance measures. Although concentrating on mobile source modeling, the authors suggested that paired and unpaired data be analyzed to satisfy the needs of both the scientist and the decision maker. The paired data approach is illustrated by Rao and Visalli in tables that stratify the data according to various meteorological classes and distance intervals. They examined the paired data for the central tendencies, not for the extremes. The authors state that the unpaired approach includes the probabilistic nature of the atmospheric model behavior, but stresses the importance of general overall tendencies and behaviour for evaluation of models. Finally, to satisfy the regulatory aspect of model evaluations, Rao and Visalli discuss in detail the use of extreme-value statistics for estimating peak concentrations.

Fox (1981) recently summarized recommendations made at a workshop in Wood Hole, Massachusetts, for model performance evaluation. The workshop participants agreed upon four areas that limit the accuracy of air quality model estimates:

- 1) The quality of the emissions data.
- 2) The quality (appropriateness or relevance to the problem) of the meteorological data.
- 3) The quality of ambient air quality measurements available for comparison.
- 4) The capability of the algorithms to reproduce natural events.

Fox suggested that the data be grouped into paired observed and predicted concentrations (most stringent grouping), peak concentrations grouped in different ways with respect to time and space, and cumulative frequency distributions. The actual statistics that Fox recommended centered on residual analysis, especially the bias, the variance of the residuals, and the gross variability of the residuals. He also noted that various correlation coefficients could be used as performance measures. However, in suggesting specific measures, Fox warned that further research is needed to establish what statistical tests are needed for the many applications of air quality models.

SECTION 4

MODEL DEVELOPMENT

As discussed in the section on validation procedures, many researchers are concerned about the quality of emissions input, meteorological input, and the methods used in calculating dispersion. These areas were addressed in the design of the alternative modeling matrix used in this study.

The benchmark model from which the alternatives were developed was the MPTER algorithm, Multiple Point Gaussian Dispersion Algorithm with Optional Terrain Adjustment (Pierce and Turner, 1980). MPTER is an air quality simulation model that is used by the EPA in regulatory applications. MPTER was especially suited for this study because actual coordinates for each monitoring site could be specified along with the physical separation between stacks. Furthermore, the author's in-depth experience with MPTER allowed for careful and expedient development of the alternative models.

In modeling for regulatory applications, the design capacity or the maximum operating capacity of resulting SO_2 emissions and source parameters are often required as model inputs. The daily and seasonal operating rates vary significantly at most coal-fired power plants. Furthermore, according to Irwin and Cope (1979), maximum surface concentrations at a power plant can occur under less than full-load conditions. Thus, for the Johnsonville and Paradise locations, hourly SO_2 emissions, stack gas temperatures, and gas exit velocities were computed for comparison to full-load conditions.

The meteorological data required for EPA regulatory applications are often selected from the NWS stations that are most representative of the site being modeled. In this study, the airport data from Nashville (BNA) were used as model inputs for the Paradise and Johnsonville sites. Evansville (EVV) surface data were also included for comparison at the Paradise site. Because the use of onsite meteorological data is preferred, the hourly average 110 m onsite wind data were used at both power plants.

An accurate estimate of dispersion is critical in air quality analysis. In this regard, much effort was made in developing the alternative models in this study. MPTER uses PG dispersion coefficients. As one alternative, Pasquill's approach for estimating buoyancy-induced-dispersion (Pasquill, 1976) was evaluated. Briggs' rural dispersion coefficients (Gifford, 1976) combined with Pasquill's buoyancy-induced-dispersion were also examined. Finally, three schemes -- Pasquill (1976), Draxler (1976), and Cramer (1976) -- that use onsite turbulence measurements were evaluated for the Johnsonville site. These schemes were reviewed in the technical section.

A matrix of model alternatives was developed for Paradise, 1976, and for Johnsonville, 1977. These matrices are shown in Table 9 and Table 10. It should be noted that the alternative models were developed with an effort made to keep each change in a technique independent of the other techniques.

TABLE 9. MODELING ALTERNATIVE MATRIX USED FOR PARADISE, 1976

Technique	Model number						
	1	2	3	4	5	6	7
<u>Emissions input</u>							
Full-load conditions	X	X					
Hourly averages			X	X	X	X	X
<u>Meteorology input</u>							
BNA airport data	X		X				
EVV airport data				X			
Onsite wind data		X			X	X	X
<u>Dispersion scheme</u>							
PG	X	X	X	X	X		
PG with buoyancy-induced-dispersion						X	
Briggs formulae with buoyancy-induced-dispersion							X

TABLE 10. MODELING ALTERNATIVE MATRIX FOR JOHNSONVILLE, 1977

[illegible]

* Bouyancy-induced-dispersion

SECTION 5

PARADISE ANALYSIS

The evaluation of the seven modeling alternatives using the hourly 1976 Paradise data was conducted for two reasons: (1) to determine the effect of each modeling alternative in predicting peak SO_2 concentrations, especially the concentrations associated with the National Ambient Air Quality Standards (NAAQS), and (2) to provide a diagnostic evaluation of each modeling alternative. The NAAQS for SO_2 specify that a site shall not exceed a 3-hour average concentration of $1300 \mu\text{g}/\text{m}^3$ and a 24-hour average concentration of $365 \mu\text{g}/\text{m}^3$ more than once a year.

Air quality models have been especially designed to predict the second-highest 3-hour and 24-hour average concentrations. Because it is difficult to statistically evaluate the performance of a model using just these two extreme values, the top 25 1-hour, 3-hour, and 24-hour average concentrations were also examined in this study so that model performance might be better assessed. For diagnostic evaluation, predicted and observed hourly concentrations for a range of meteorological conditions were compared to explore the strengths and weaknesses of the alternative modeling techniques.

PEAK CONCENTRATIONS

Second-Highest 3-Hour Concentrations

The second-highest predicted and observed 3-hour average SO_2 concentrations from hourly 1976 Paradise data are listed for each receptor in Table 11. The highest second-highest concentration, $1036 \mu\text{g}/\text{m}^3$, was observed at receptor nine. The highest second-high 3-hour average concentration is predicted to occur at receptor nine by only models 2 and 4 with predictions of $1330 \mu\text{g}/\text{m}^3$ and $649 \mu\text{g}/\text{m}^3$.

The conditions resulting in the second-highest 3-hour concentrations at receptor eight are noted in Table 12. Receptor eight was selected for examination because of the high predictions and observations associated with it as compared to the other receptors. The meteorological conditions associated with the second-highest observed 3-hour concentrations at receptor eight were characterized by light, persistent winds and unstable conditions. The flow vectors, observed from the 110 m onsite meteorological tower during the three hours, were 25° off an azimuth centered towards receptor eight. In contrast, the BNA flow vectors used in model 1 resulted in an impact of $3107 \mu\text{g}/\text{m}^3$ and were only 6° off the centerline azimuth. The meteorological conditions during this 3-hour period were described as very unstable (A-stability) with a wind speed of 1 m/s.

Very unstable, light wind conditions were also associated with second-highest predicted 3-hour concentrations for models 2, 5, 6, and 7. In comparing the dispersion schemes, the use of Briggs coefficients in model 7 resulted in concentrations that averaged 30 percent less

TABLE 11. SECOND-HIGHEST PREDICTED AND OBSERVED 3-HOUR AVERAGE SO₂ CONCENTRATIONS AT EACH PARADISE RECEPTOR DURING 1976*

Receptor site	Obs.	1	2	Model number		5	6	7
				3	4			
1	479 (284,18)	554 (284,15)	324 (241,15)	321 (284,15)	204 (263,12)	167 (263,15)	238 (263,15)	227 (263,15)
2	583 (286,15)	486 (307,12)	354 (267,12)	290 (307,12)	304 (255,15)	255 (257,15)	253 (257,12)	252 (335,12)
3	836 (125,12)	1062 (131,12)	1005 (125,15)	439 (284,15)	473 (226,12)	420 (202,15)	418 (210,15)	410 (210,15)
4	461 (240,12)	649 (257,12)	878 (323,15)	332 (284,15)	341 (226,12)	260 (263,15)	258 (263,15)	258 (263,15)
5	531 (323,15)	559 (257,12)	689 (263,15)	280 (307,15)	311 (255,12)	189 (263,15)	226 (335,12)	208 (335,12)
6	766 (223,18)	559 (147,18)	1003 (201,15)	296 (75,12)	361 (340,15)	585 (201,15)	581 (201,15)	597 (201,15)
7	940 (24,12)	1221 (194,12)	1038 (142,15)	657 (194,12)	403 (205,09)	592 (219,18)	599 (219,18)	609 (219,18)
8	1010 (82,15)	1307 (143,15)	1142 (104,12)	498 (200,15)	226 (258,15)	626 (201,12)	639 (237,12)	469 (237,12)
9	1036 (195,15)	919 (96,15)	1330 (182,12)	446 (96,15)	649 (194,12)	594 (309,12)	637 (309,12)	642 (309,12)
10	1010 (306,15)	950 (159,15)	961 (160,12)	444 (66,15)	600 (230,12)	533 (102,18)	536 (102,18)	540 (102,18)
11	697 (96,15)	888 (201,15)	1090 (240,15)	495 (201,15)	716 (223,15)	571 (256,12)	572 (256,12)	573 (256,12)
12	679 (159,12)	1055 (187,12)	1178 (268,15)	610 (187,12)	496 (188,18)	754 (268,15)	780 (268,15)	745 (268,15)

*Numbers in parentheses indicate day and ending hour of occurrence. Concentrations in units of $\mu\text{g}/\text{m}^3$.

TABLE 12. HOURLY CONDITIONS RESULTING IN THE SECOND-HIGHEST PREDICTED AND OBSERVED 3-HOUR AVERAGE SO₂ CONCENTRATIONS AT PARADISE RECEPTOR EIGHT*

Parameter	Observed		Model 1		Model 2	Models 5, 6, and 7	
Concentration ($\mu\text{g}/\text{m}^3$)	1045	940	1045	815	857	2569	952 - 1298 456 - 680
Julian day, hour	82,13	82,14	82,15	143,13	104,11	104,12	237,11 237,12
Emission rate (kg/s)	14.3	14.1	14.2	22.2	22.2	22.2	5.9 5.9
BNA meteorology							
Wind speed (m/s)	3.1	2.1	3.6	3.1	1.0		
Flow vector (°)#	318	258	232	293	295		
Mixing height (m)	1716	1957	1957				
Stability class	B	B	C	B	A	A	1046 1228 A
EW stability class	C	B	C				
Onsite meteorology							
110 m Wind speed (m/s)	2.7	2.2	2.7		3.3	3.5	2.3 2.3
110 m Flow vector (°)#	277	276	273		286	294	295 289

*Only the hours during which the concentrations exceeded 50 $\mu\text{g}/\text{m}^3$ are reported above.
 Data not shown were not used in the model application.
 #Receptor eight is located at an azimuth of 301°.

than the concentrations predicted with the two models using PG dispersion coefficients. The rather large differences in concentrations were found to occur, however, at only this receptor site.

The highest second-high 3-hour concentration was overpredicted by the models using full-load emissions data, models 1 and 2. The models using full-load emissions data also tended to overpredict the second-high concentrations at the other receptor sites.

In contrast, substantial underpredictions were noted with the models using hourly average emission parameters, models 3 to 7. By comparing the results of model 1 to model 3 and model 2 to model 5, the effect of emissions was isolated. This comparison showed that by changing from full-load emissions to hourly average emissions that modeled concentrations were reduced by approximately 50 percent.

When only the meteorological data or the dispersion schemes were changed, only small differences in the second-high 3-hour concentrations were noted. A comparison between the models indicated that the concentrations varied between receptors, but there was not any evidence that differences between the models varied as a function of distance from the source for either the onsite meteorological data or the airport data. Differences in dispersion coefficient schemes, as seen by comparing models 5, 6, and 7, were on the order of ten percent. It does appear from Table 11 that the model not using buoyancy-induced-dispersion resulted in lower overall concentrations than the two models using buoyancy-induced-dispersion.

Second-Highest 24-Hour Concentrations

The second-highest observed and predicted 24-hour average SO_2 concentrations with the 1976 Paradise data are listed in Table 13. The highest of these concentrations, $335 \mu\text{g}/\text{m}^3$, was observed at receptor ten, and this concentration was at least $70 \mu\text{g}/\text{m}^3$ higher than the concentrations predicted by any of the seven models.

The conditions resulting in the second-highest 24-hour concentration at receptor ten are listed in Table 14. Only those hours in a 24-hour period when concentrations were greater than $10 \mu\text{g}/\text{m}^3$ are listed. The observed second-highest 24-hour concentration at receptor ten was reported on day 321 when concentrations greater than $50 \mu\text{g}/\text{m}^3$ were reported for 20 hours. Stability classes observed from airport meteorological data during these hours ranged from very stable (G-stability) to slightly unstable (B-stability). Also during day 321, the onsite 110 m level wind speeds were moderate at night and less than 2 m/s during the day. In general, onsite wind directions were directed towards the southwest sector in the general direction of receptor ten. The 110 m flow vector during the hours of the high observed concentrations was oriented 30° off the azimuth centered at receptor ten.

In contrast to the observed second-highest 24-hour concentrations, only two to four hours of data contributed significantly to the modeled second-highest 24-hour average concentrations. With model 1, stability classes A, B, and C, and flow vectors within five degrees of centerline contributed to the highest three hours of predicted concentrations. Unstable meteorological conditions were also noted in the predictions by models 5, 6, and 7.

TABLE 13. SECOND-HIGHEST OBSERVED AND PREDICTED 24-HOUR AVERAGE SO₂ CONCENTRATIONS AT EACH PARADISE RECEPTOR DURING 1976*

Receptor	Observed	Model number						
		1	2	3	4	5	6	7
1	118 (366)	69 (284)	42 (241)	40 (284)	29 (263)	21 (323)	35 (323)	38 (323)
2	109 (366)	61 (307)	74 (257)	36 (307)	52 (241)	53 (257)	53 (257)	51 (257)
3	205 (96)	155 (181)	233 (165)	83 (267)	86 (226)	75 (210)	82 (170)	94 (170)
4	82 (288)	83 (286)	119 (323)	42 (284)	54 (266)	48 (263)	51 (263)	51 (263)
5	104 (323)	72 (307)	129 (323)	43 (307)	54 (311)	41 (263)	42 (263)	42 (263)
6	157 (121)	108 (169)	215 (201)	40 (292)	56 (269)	110 (82)	115 (82)	108 (223)
7	218 (14)	251 (194)	159 (142)	140 (194)	86 (190)	89 (219)	89 (219)	91 (219)
8	205 (121)	166 (143)	184 (201)	62 (200)	37 (136)	83 (130)	83 (237)	80 (292)
9	224 (366)	159 (265)	228 (183)	71 (124)	80 (199)	129 (183)	132 (183)	128 (183)
10	335 (321)	191 (159)	158 (97)	82 (98)	107 (229)	73 (215)	76 (215)	77 (215)
11	135 (82)	149 (201)	238 (252)	77 (252)	128 (169)	146 (252)	145 (252)	140 (252)
12	157 (128)	210 (234)	176 (234)	121 (242)	84 (160)	107 (268)	115 (268)	110 (268)

*Numbers in parentheses indicate the day of occurrence.
Concentrations in $\mu\text{g}/\text{m}^3$.

TABLE 14. HOURLY SO₂ CONCENTRATIONS AND METEOROLOGICAL CONDITIONS ASSOCIATED WITH THE SECOND-HIGHEST OBSERVED AND MODELED 24-HOUR AVERAGE CONCENTRATIONS AT PARADISE RECEPTOR TEN FOR 1976#

Observed (Julian day 321)									
Hour	Observed concentration ($\mu\text{g}/\text{m}^3$)	Emission rate (kg/s)	Onsite		BNA airport				
			Wind speed (m/s)	Flow vector ($^{\circ}$)	Wind speed (m/s)	Flow vector ($^{\circ}$)	Stability class	Mixing height (m)	
01*									
02	157	15.3	6.5	230	2.6	125	F	-	
03*									
04*									
05	104	15.3	3.6	264	2.6	119	F	-	
06	157	15.3	4.7	287	3.1	133	F	-	
07	104	15.3	4.5	307	2.6	136	E	-	
08	104	15.3	4.9	308	2.1	156	D	258	
09*									
10*									
11*									
12	313	14.9	1.6	237	3.1	206	C	945	
13	1149	15.0	1.3	267	3.6	233	C	1116	
14	1724	15.0	1.4	264	3.6	186	C	1288	
15	1228	14.8	1.2	277	5.1	222	D	1288	
16	653	14.8	0.9	255	3.1	230	D	1288	
17	339	14.9	1.3	196	1.5	208	E	-	
18	418	14.9	2.2	204	2.1	194	F	-	
19	235	15.1	3.6	205	2.1	178	F	-	
20	131	15.1	4.7	221	2.1	187	F	-	
21	156	14.6	4.1	236	2.6	173	F	-	
22	287	14.4	2.1	279	1.0	170	G	-	
23	313	14.4	2.1	288	1.0	169	G	-	
24	313	14.4	3.8	312	2.1	033	F	-	

continued

TABLE 14 (continued).

Model 1 (Julian day 159)						
Hour	Modeled concentration ($\mu\text{g}/\text{m}^3$)	BNA Airport			BNA Airport	
		Wind speed (m/s)	Flow vector ($^\circ$)	Stability class	Stability class	Mixing height (m)
01-10*						
11	315	4.1	250	B		1448
12*						
13	408	2.1	253	A		1865
14	1541	2.6	238	B		2073
15	901	4.1	243	C		2073
16-24*						
Models 5, 6, and 7 (Julian day 215)						
Hour	Modeled concentrations ($\mu\text{g}/\text{m}^3$)	Emission rate (kg/s)	Onsite		BNA Airport	
			Wind speed (m/s)	Flow vector ($^\circ$)	Stability class	Mixing height (m)
01-07*						
08	725 721 728	14.2	5.9	240	B	574
09*						
10	126 131 127	14.1	3.5	225	B	954
11*						
12*						
13	813 864 859	13.9	5.1	238	C	1525
14-24*						

#Receptor ten is located at an azimuth of 238°.

*Only the hours during which the concentrations exceeded 100 $\mu\text{g}/\text{m}^3$ are reported above.

The flow vectors for these three models were also within five degrees of the centerline azimuth.

As with the second-highest 3-hour results, the models using full-load emissions data overpredicted the second-highest 24-hour concentrations. The overpredictions for the 24-hour averaging period, however, were not as large as the overpredictions for the 3-hour averaging period.

Again, the models using hourly average emissions data, models 3-7, underpredicted the observed concentrations by about a factor of two. A comparison of the meteorological input alternatives and the dispersion schemes showed results that were similar to the 3-hour analysis. The use of onsite versus airport meteorological data did not show any definite trend. Among the dispersion schemes, the results agreed within about ten percent. However, it does appear from Table 13 that models 6 and 7 yielded slightly higher concentrations than model 5.

Geometric Mean Concentrations

The models' ability to predict the top 25 1-, 3-, and 24-hour average concentrations was also considered. From predictions of each model, the geometric means of the top 25 concentrations were computed. Data from receptors one, two, four, and five were eliminated from further analysis because less than 40 percent of the hours during 1976 were available for these sites. The modeled geometric mean concentrations for each averaging time and for each receptor were plotted against the geometric mean concentrations for the top 25 observations. These plots are shown in Figures 12 through 18.

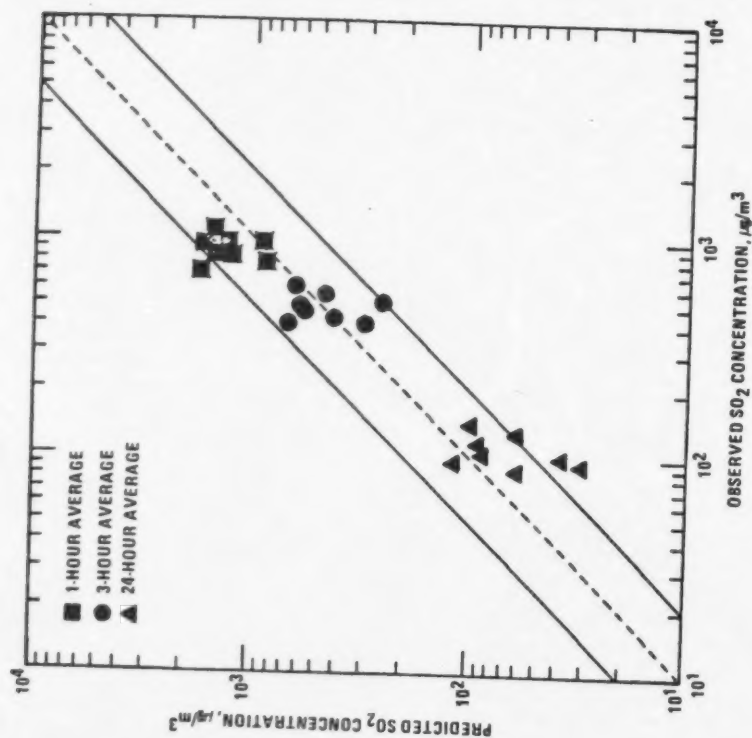


Figure 12. Comparison of model 1 and observed geometric means of the top 25 1-, 3- and 24-hour average concentrations at Paradise, KY, during 1976.

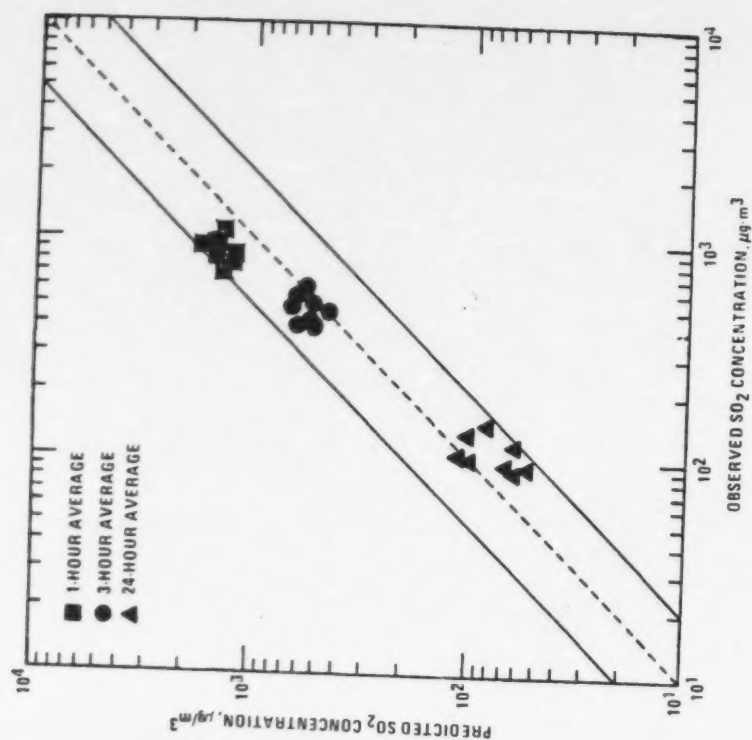


Figure 13. Same as Figure 12, except for model 2.

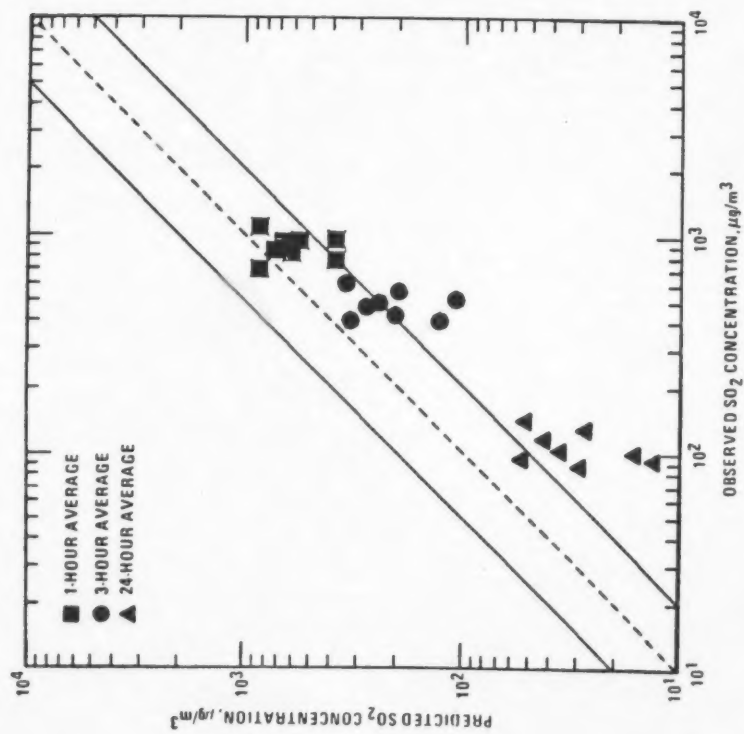


Figure 14. Same as Figure 12, except for model 3.

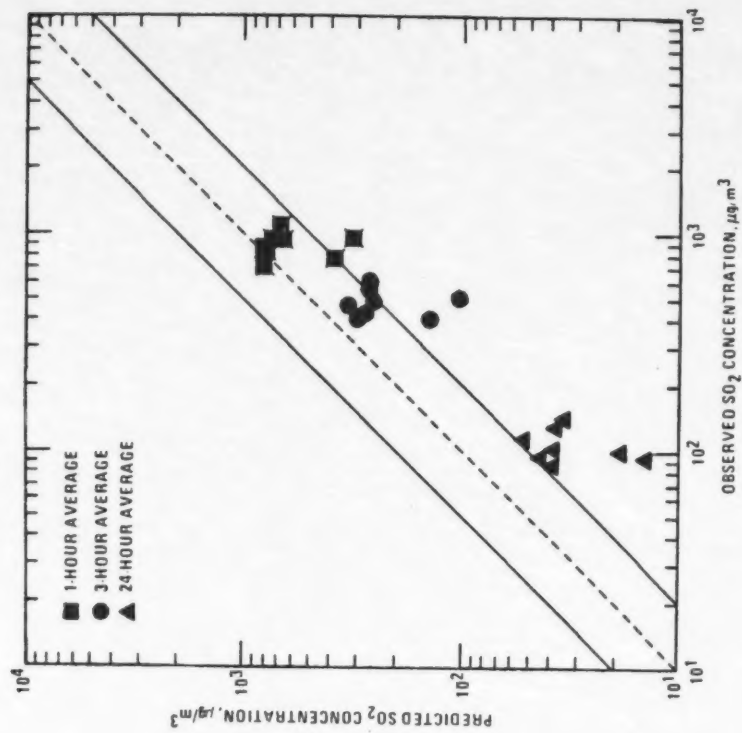


Figure 15. Same as Figure 12, except for model 4.

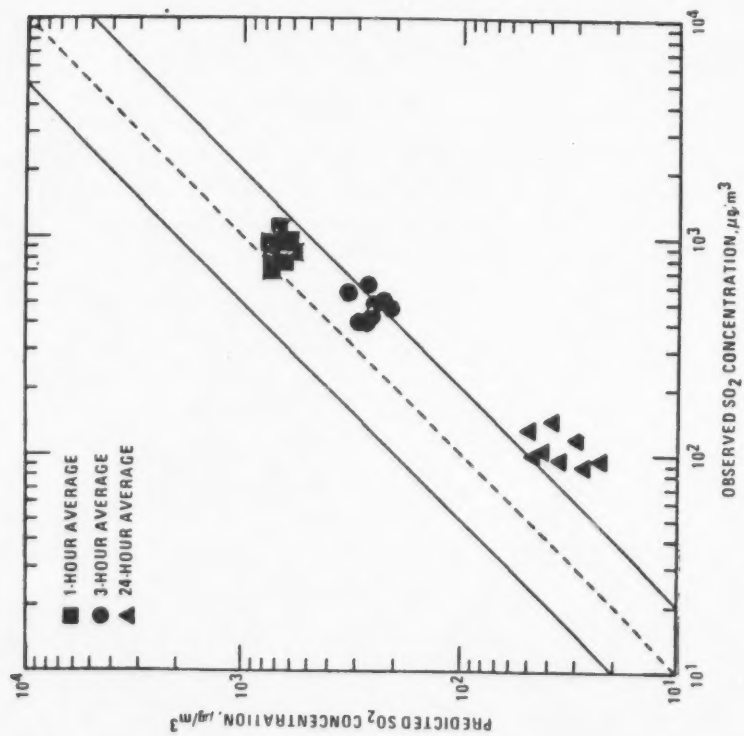


Figure 16. Same as Figure 12, except for model 5.

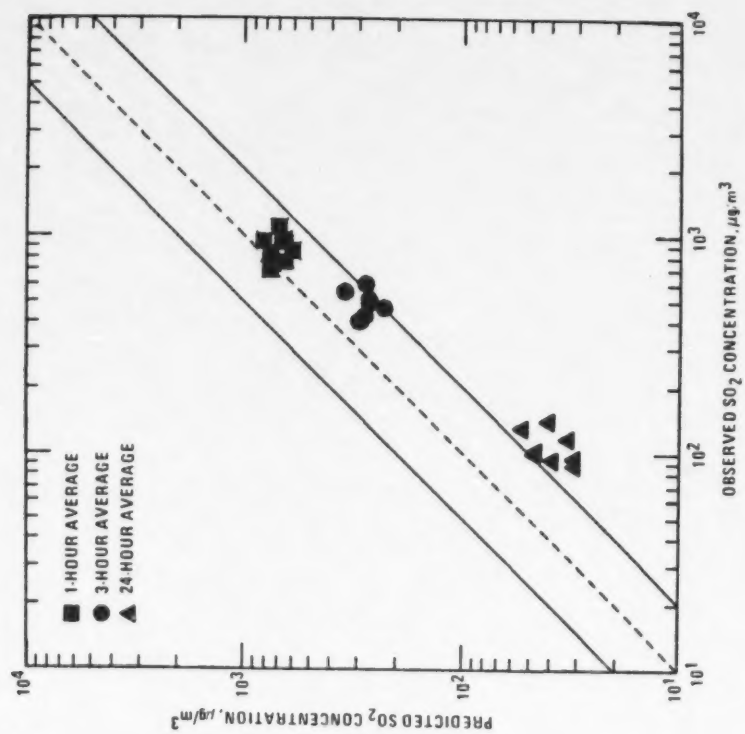


Figure 17. Same as Figure 12, except for model 6.

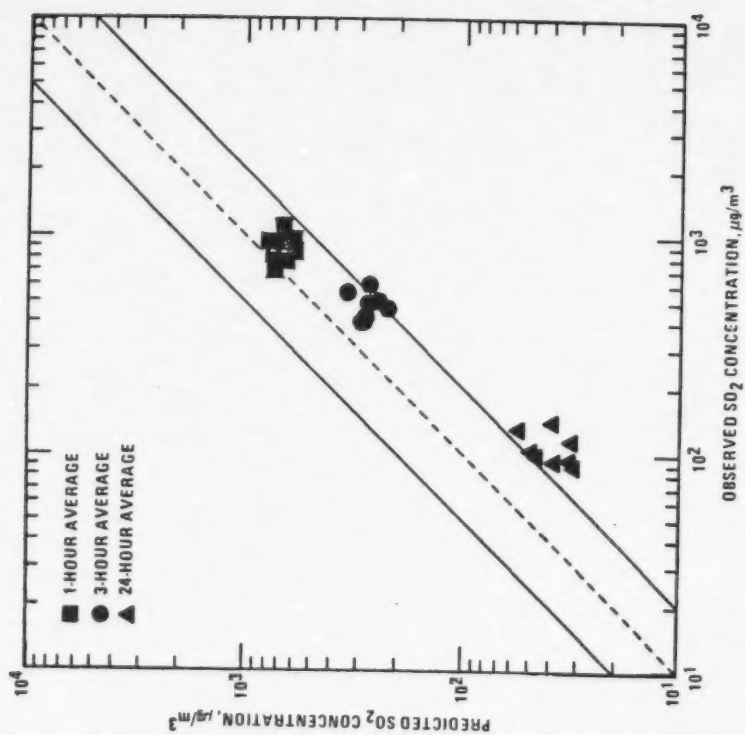


Figure 18. Same as Figure 12, except for model 7.

The geometric mean concentrations were underpredicted for all averaging times by all models using hourly average emissions data. The underprediction appears to increase with greater averaging time. By comparing those values that were within a factor of two, the best comparisons were achieved with model 2. Models 3 and 4 compared poorly to the observations. Although the magnitude of concentrations was similar to that for model 2, model 1 is characterized in Figure 13 by greater overpredictions for 1-hour values and by greater underpredictions for the 24-hour values. The predictions from models 5, 6, and 7 agreed closely with each other, although they significantly underpredicted the observed concentrations.

DIAGNOSTIC EVALUATION

Pollution Roses

To investigate the uncertainty of wind directions in predicting high surface concentrations, pollution roses were plotted for the top 25 observed hourly concentrations at each Paradise receptor using the 110 m level onsite wind directions. Figure 19 shows the relative frequency by sector of the top 25 concentrations. Each pollution rose was centered towards the power plant. Many hourly concentrations were reported having wind directions that were displaced more than 45° off the azimuth centered towards the power plant. In contrast, the top 25 predicted hourly concentrations occurred with assumed wind directions that were within 10° of the azimuth centered towards the power plant.

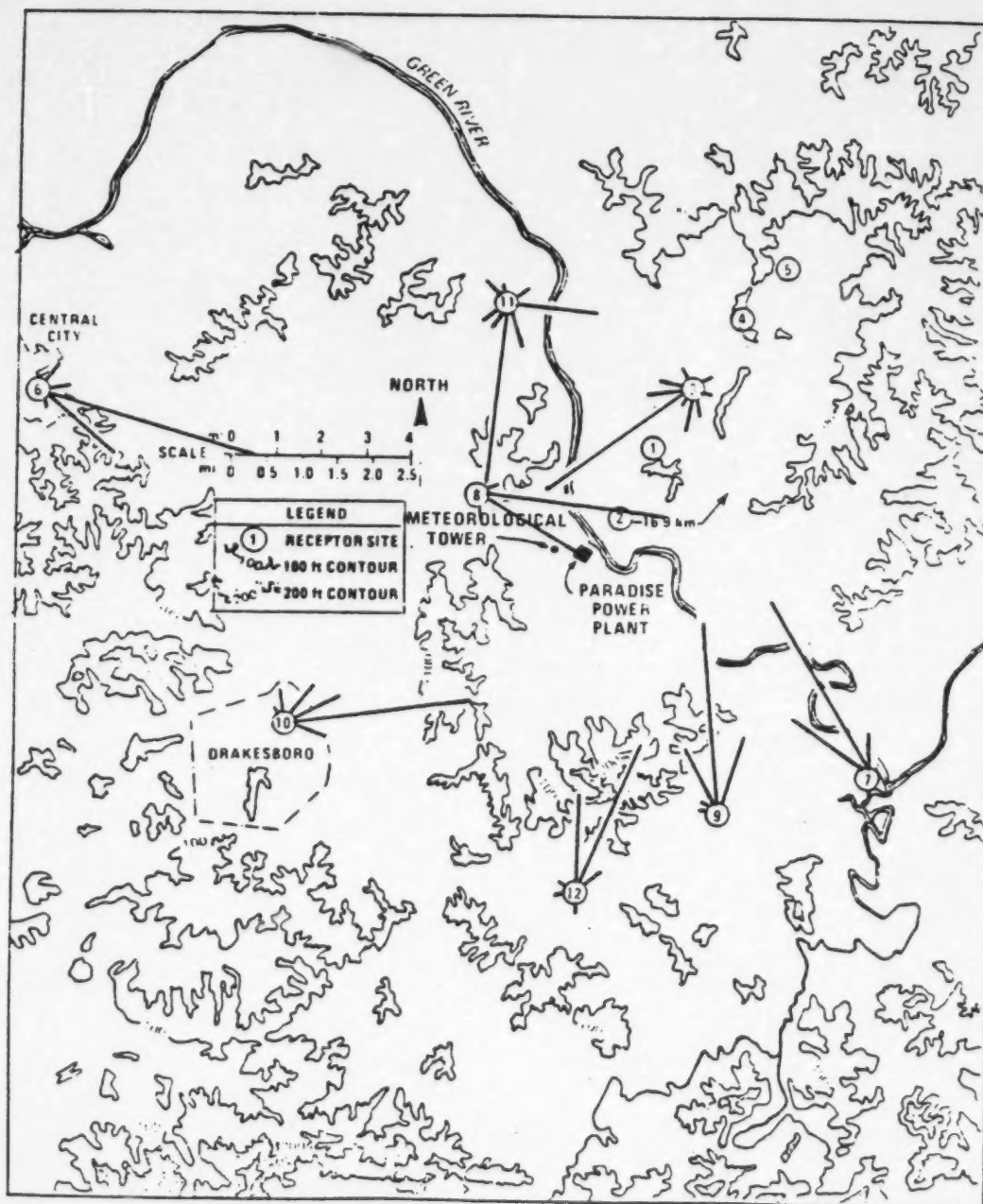


Figure 19. Pollution roses of the top 25 hourly (observed at each receptor) SO₂ concentrations at Paradise using 110 m wind direction data from the onsite meteorological tower.

Correlation Coefficients

Up to this point, comparisons of paired observations and predictions have not been discussed, because studies have shown that the Gaussian plume dispersion model poorly reproduces the concentrations observed on a short-term basis (for example, Mills, 1977). Nevertheless, Pearson correlation coefficients were computed for each pair of valid hourly observed and modeled concentrations at each receptor. These correlation coefficients are listed in Table 15.

As expected, the computed Pearson correlation coefficients were quite low. In fact, a check for significance at the 95 percent level showed that most correlations for models using airport data (models 1, 3, and 4) could not be rejected from the null hypothesis of no correlation. Predictions from model 2 were found to be significantly greater than zero correlation at every receptor site.

Meteorological Stratification

In an effort to compare the average hourly modeled concentrations under a range of meteorological conditions, the hourly concentrations were stratified by meteorological conditions using the following criteria:

- 1) Three groups corresponding to stability classes B, C, and D were defined as those hours when both EVV and BNA reported the same stability class. (Not enough data were available for an A-stability grouping.)
- 2) An "unstable group" was developed from those hours when both EVV and BNA reported A, B, or C stability.

TABLE 15. PEARSON CORRELATION COEFFICIENTS COMPUTED FROM VALID HOURLY
SO₂ CONCENTRATIONS PREDICTED AND OBSERVED AT PARADISE DURING 1976

Receptor	1	2	3	Model 4	5	6	7
3	0.07	0.08*	0.06	0.05	0.07	0.07	0.07
6	0.03	0.24*	0.03	0.07	0.24*	0.24*	0.23*
7	0.10*	0.09*	0.10*	0.09*	0.09*	0.10*	0.09*
8	0.01	0.14*	0.01	0.11*	0.16*	0.19*	0.19*
9	0.06	0.10*	0.06	0.07	0.10*	0.11*	0.11*
10	0.06	0.09*	0.05	0.04	0.08*	0.09*	0.09*
11	0.02	0.10*	0.02	0.07	0.10*	0.11*	0.11*
12	0.10*	0.17*	0.09*	0.17*	0.14*	0.15*	0.15*

*Reject the null hypothesis of no correlation at the five percent level of significance.

The observed and modeled hourly concentrations were further stratified to include only those cases when the wind direction, reported from the 110 m tower, was directed in $22\frac{1}{2}^{\circ}$ sector centered towards the receptor. This stratification into B, C, D, and unstable groups was used on four receptors that represented a range of distances: receptor eight (3.38 km), receptor three (4.59 km), receptor eleven (6.05 km), and receptor seven (8.53 km).

Figures 20-24 depict the results from the four receptors. Figures 20, 21, 22, and 23 show the effect the three stability groups and the unstable group at each receptor. Figure 24 shows the change in prediction ability as a function of distance. The mean fractional error (MFE) was computed for each model using the following equation:

$$MFE = 2 (P - O) / (P + O)$$

where P is the mean predicted concentration for all cases in a stratification, and O is the mean observed concentration for that stratification. The above expression is logarithmically unbiased and follows that used by Gryning and Lyck (1980) in making similar comparisons.

All models tended to underestimate concentrations as the stability class increased, with all models underpredicting the mean concentrations during D-stability. In fact, most predicted concentrations were zero during D-stability.

Changing from an model using airport meteorological data to a model using onsite wind data, as seen by comparing model 1 to model 2 and model 3 to model 5, usually resulted in an increase of mean predicted concentrations. However, this did not necessarily mean an

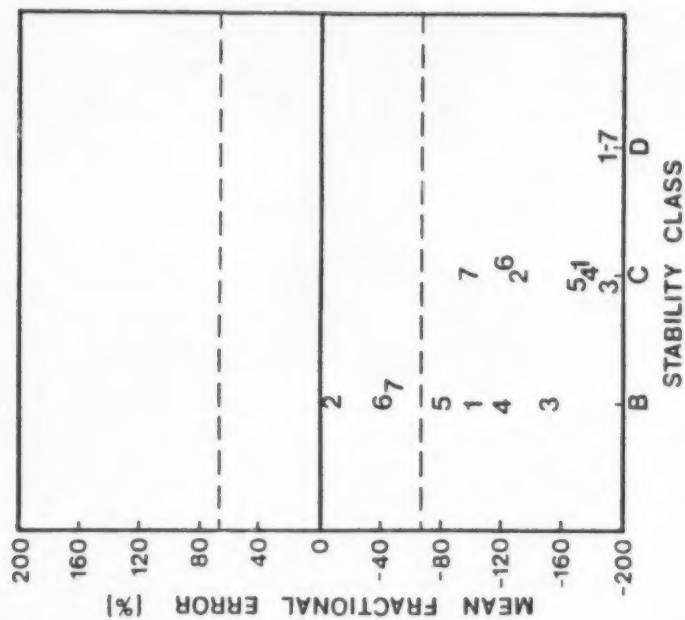


Figure 20. Mean fractional errors computed for each alternative model (numbered from 1 to 7) and stratified by stability class at Paradise receptor eight ($x = 3.4$ km).

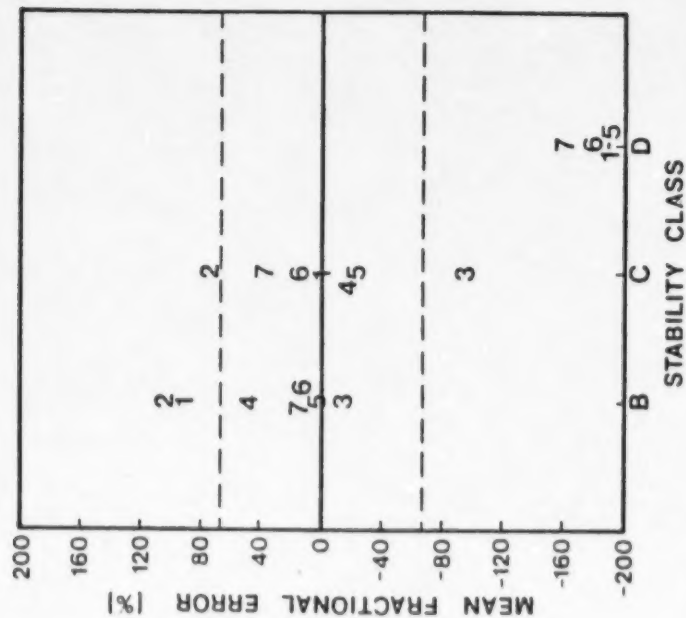


Figure 21. Same as Figure 20, except for receptor three ($x = 4.7$ km).

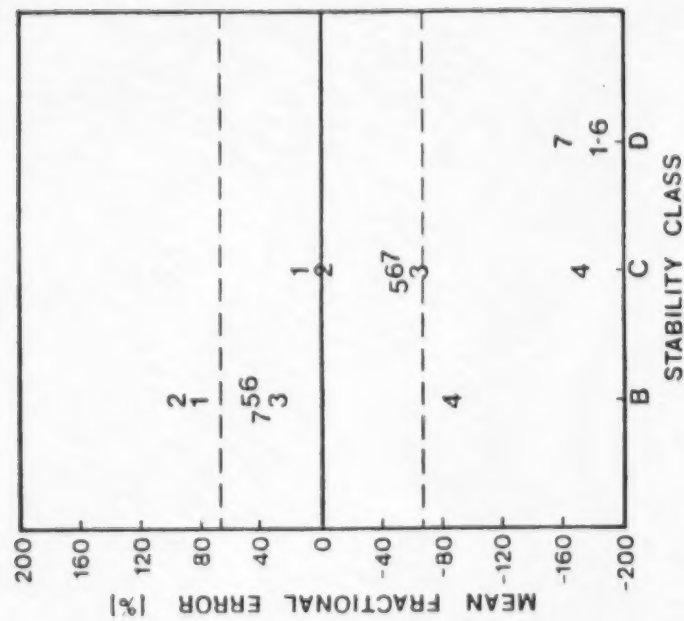


Figure 22. Same as Figure 20, except for receptor eleven ($x = 6.1$ km).

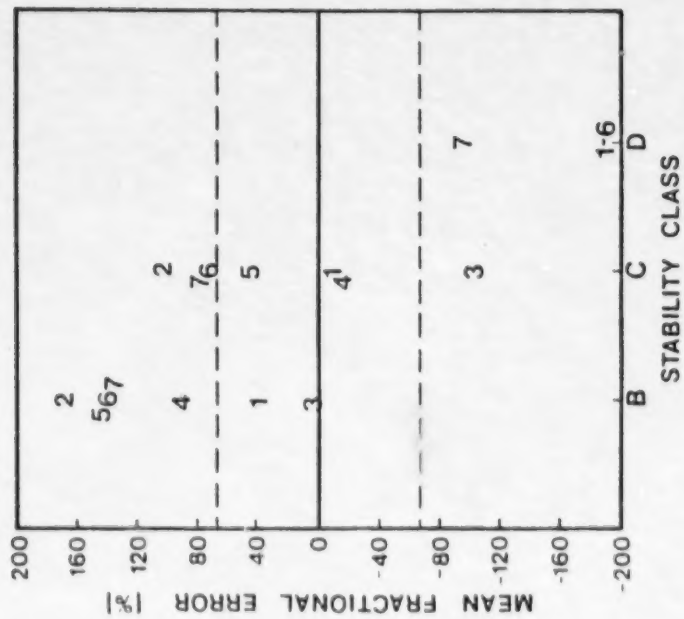


Figure 23. Same as Figure 20, except for receptor seven ($x = 8.5$ km).

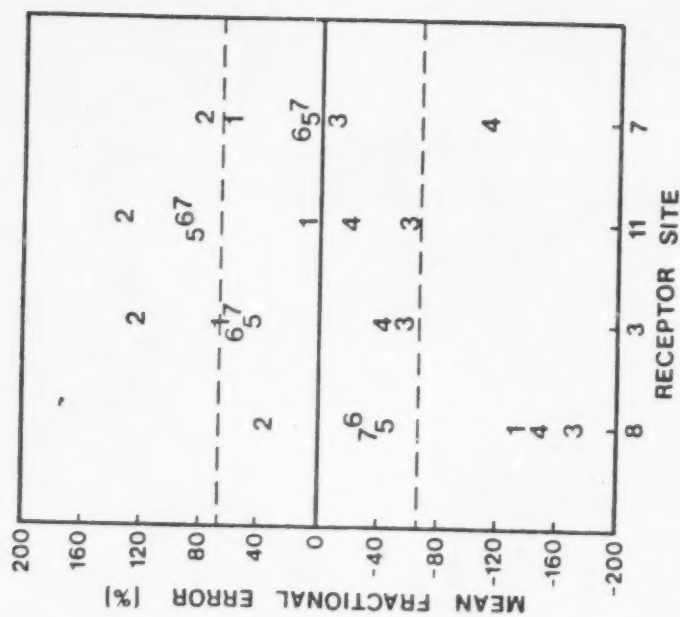


Figure 24. Mean fractional errors computed for each alternative model (numbered from 1 to 7) for unstable conditions at Paradise receptors 8, 3, 11, and 7.

improvement in the MFE. Comparing the model using BNA meteorological data to the model using EVV data, model 3 to model 4, showed that model 4 resulted in lower mean concentrations. The MFEs among the models using different dispersion schemes, models 5, 6, and, 7, were within ten percent as reflected by the clustering in the figures.

Comparing the models using different emissions data, models 1 to model 3 and model 2 to model 5, showed that concentrations were reduced by about 50 percent.

All models underestimated the mean concentration at the receptor closest to the power plant, which reported a mean observed concentration of $235 \mu\text{g}/\text{m}^3$ during B-stability. At the remaining receptors, the models either underestimated or overestimated the mean concentrations for the B and C stability classifications. All models tended to underpredict concentrations near the source and tended to overpredict concentrations at the more distant receptors.

For the MFEs computed for the unstable group, models 3 and 4 underpredicted the mean concentrations at all receptors. The model using full-load emissions and onsite meteorology, model 2, overpredicted the mean concentration at all receptors. Models 1, 5, 6, and 7 both underpredicted and overpredicted concentrations under the unstable criteria. The MFEs computed for models 5, 6, and 7 compared fairly closely.

SECTION 6

PARADISE DISCUSSION

In analyzing the Paradise modeling results, the performance of the modeling alternatives in their prediction of peak concentrations was examined. In addition, attempts were made to gain some insight on the reasons for model performance (or lack thereof). Finally, the modeling results were stratified according to stability class to assess the performance of the various modeling alternatives.

PEAK CONCENTRATIONS

Similar trends in model performance were evident from the prediction of both the second-highest 3-hour and the second-highest 24-hour average SO_2 concentrations. In general, the models using full-load emissions data were more accurate in their prediction of peak concentrations. The alternatives using hourly emissions data underpredicted the second-highest 3-hour and 24-hour average concentrations by about 50 percent. The differences in concentrations resulting from the use of alternative dispersion schemes and alternative meteorological data input were small in comparison. The three dispersion schemes -- PG curves, PG curves with buoyancy-induced-dispersion, and Briggs rural interpolation formulae -- produced results that were generally within ten percent of each other. Although the differences at individual receptors due to different meteorological input were as large as 50 percent, the results averaged over the receptor network were quite similar. The values obtained with the geometric mean concentrations further supported this tendency.

The modeling framework was initially developed under the assumption that the models using hourly emissions data would "outperform" the "conservative" models using full-load emissions data. Initial modeling results did not confirm this assumption. It was then supposed that an error existed in either the hourly emissions data or the SO₂ observations. The hourly emissions data were subsequently checked with data supplied by the Tennessee Valley Authority (TVA). Therefore, the hourly emissions parameters used in this study are believed to be valid. In addition, the TVA maintained a quality assurance program to validate their SO₂ measurements. Nevertheless, it is recommended that additional work could be performed by comparing the SO₂ measurements to meteorological conditions and reported emissions to further validate the SO₂ concentration data.

DIAGNOSTIC EVALUATION

From an examination of the meteorological conditions that produced the peak modeled concentrations, it became apparent that the wind direction was a critical model parameter. This is not too surprising, because a shift in the plume centerline of only two degrees can reduce the concentration at the surface by as much as 50 percent. In contrast, when peak concentrations were measured, the reported onsite wind direction was much as 30° off an azimuth centered towards the receptor. The uncertainty in determining the plume centerline helps to explain why that even when onsite wind data are used, predictions of short-term concentrations are not improved.

When comparing the models using onsite meteorological data with those using airport meteorological data, some improvement was noted in the Pearson correlation coefficients. Although the coefficients for all models were low (a fact that further strengthens the belief that hour-to-hour conditions can not be simulated with much accuracy), the models using onsite meteorological data resulted in similar correlations. Also, these correlations were larger at all the receptors than the correlations computed for the models using airport meteorological data. Although the use of onsite meteorological data yielded apparently better correlations, the improvement did not prove to be significantly better in this study.

The computation of mean fractional errors (MFEs) further helped to diagnose the performance of the models for a range of meteorological conditions. The most striking feature of the MFE analysis was the tendency of all models to underpredict as the stability was increased. In fact, the concentrations observed during D-stability were significantly underpredicted. Furthermore, much scatter in the other stability classes was also apparent. These results indicate that discrete stability classifications did not reflect the hour-to-hour changes in atmospheric dispersion. It also suggests that the availability of onsite turbulence data might provide a more accurate measure of dispersion as suggested by Hanna, et al. (1977).

Other trends that were evident in MFE analysis corresponded to the results reported for the peak concentrations. As expected, the models using full-load emissions data predicted higher average concentrations than the models using hourly emissions data. From this

analysis, however, it was not clear whether the use of full-load emissions data was a superior predictive tool. It should be noted that the model using hourly emissions data and airport meteorological data underpredicted concentrations at all receptors.

The MFEs computed with the models using the three different dispersion schemes were again in close agreement. The results seem to be due to the relatively small changes in dispersion that resulted at the selected receptors and stability classes. Unfortunately, not enough data were available for A-stability to quantitatively assess the differences associated with the PG and Briggs dispersion coefficients. Further analyses should include more data on A-stability and should include measurements from receptor sites less than 1.5 km from the emissions source.

From the MFE analysis, there was not a clear relationship of model performance as a function of downwind distance. This could be due to orientation of the receptors around the Paradise power plant. Further research should include studies where receptors are oriented in the same direction. Tracer studies would be ideally suited for this type of analysis.

SECTION 7

JOHNSONVILLE ANALYSIS

Predictions from the 11 alternative models using 1977 hourly data were compared to hourly SO_2 concentrations measured at the 11 receptors around the Johnsonville power plant. An objective of this comparison was to evaluate the models' ability to predict peak concentrations, especially those concentrations relative to the NAAQS for SO_2 . Another objective was to diagnostically evaluate the models' performance for a range of meteorological conditions.

PEAK CONCENTRATIONS

Second-highest 3-hour Concentrations

Because the secondary NAAQS for SO_2 states that a concentration of $1300 \mu\text{g}/\text{m}^3$ is not to be exceeded more than once per year during a 3-hour period, the second-highest observed and predicted 3-hour average concentrations were examined and are listed in Table 16. The conditions that resulted in the predicted and observed 3-hour concentrations at receptor six are presented in Table 17. Receptor six was selected for examination because it yielded the highest observed second-highest 3-hour concentration.

The alternatives for emissions can be examined in Table 16. Changing the emissions from full-load to daily or hourly average emissions, as seen by comparing models 1, 3, and 4, reduced the concentrations on average by 20 percent. Comparison of the model using daily emissions (model 3) to the model using hourly average emissions (model 4) showed only small differences.

TABLE 16. THE SECOND-HIGHEST OBSERVED AND MODELED 3-HOUR AVERAGE SO₂ CONCENTRATIONS AT EACH JOINSONVILLE RECEPTOR DURING 1977*

Receptor	Observed	Model 1	Model 2	Model 3	Model 4	Model 5	Model 6	Model 7	Model 8	Model 9	Model 10	Model 11
1	1724 (117,09)	1521 (336,12)	1521 (336,12)	1049 (179,09)	1110 (179,09)	1110 (179,09)	1167 (33,15)	1184 (125,12)	1188 (125,12)	1917 (189,18)	1312 (220,12)	1695 (67,12)
2	1263 (342,06)	1551 (122,15)	1460 (48,15)	1175 (122,15)	1229 (122,15)	1211 (294,12)	1374 (240,15)	1374 (240,15)	1375 (109,12)	1715 (108,09)	1263 (109,12)	1173 (80,12)
3	627 (106,12)	1833 (270,15)	1833 (270,15)	1371 (270,15)	1441 (270,15)	1441 (270,15)	1205 (83,12)	1264 (215,18)	1185 (215,18)	1446 (282,09)	1536 (152,12)	1870 (215,18)
4	740 (76,06)	1083 (187,12)	975 (247,12)	708 (131,09)	757 (131,09)	607 (187,12)	902 (83,12)	899 (83,12)	894 (83,12)	961 (83,12)	848 (83,12)	765 (83,12)
5	1271 (215,15)	1304 (226,06)	1304 (226,06)	1071 (216,03)	1116 (109,12)	1116 (109,12)	1072 (318,15)	1125 (260,09)	1072 (318,15)	2242 (260,09)	1096 (177,12)	909 (177,12)
6	1846 (265,15)	2177 (223,12)	2177 (223,12)	1521 (223,12)	1487 (223,12)	1487 (223,12)	1687 (125,12)	1686 (125,12)	1702 (42,15)	2703 (125,12)	1929 (179,15)	2614 (33,15)
7	1593 (101,12)	1913 (97,12)	1913 (97,12)	1465 (219,09)	1406 (219,09)	1406 (219,09)	1407 (106,15)	1405 (106,15)	1369 (106,15)	1867 (106,15)	1083 (173,12)	1474 (106,15)
8	984 (19,12)	585 (10,03)	585 (10,03)	458 (39,15)	448 (29,12)	448 (29,12)	640 (29,12)	672 (29,12)	672 (29,12)	631 (29,12)	554 (29,15)	465 (30,12)
9	940 (322,15)	1172 (287,12)	1177 (287,12)	1080 (315,12)	1135 (315,12)	1135 (315,12)	1219 (145,12)	1308 (145,12)	1199 (145,12)	1338 (36,12)	1320 (36,12)	1068 (145,12)
10	1219 (22,12)	872 (108,16)	872 (108,16)	643 (208,09)	616 (208,15)	616 (208,15)	737 (308,24)	866 (146,12)	705 (308,24)	697 (208,09)	780 (195,18)	390 (132,09)
11	1210 (317,15)	1606 (283,15)	1480 (154,09)	985 (277,15)	1319 (99,12)	1089 (154,09)	1457 (293,12)	1579 (317,12)	1527 (293,12)	2398 (280,09)	1514 (246,12)	1749 (293,12)

*Numbers in parentheses indicate the day and ending hour of occurrence.
Concentrations reported in $\mu\text{g}/\text{m}^3$.

TABLE 17. HOURLY CONDITIONS RESULTING IN THE SECOND-HIGHEST OBSERVED AND MODELED 3-HOUR AVERAGE SO₂ CONCENTRATIONS AT JOHNSONVILLE RECEPTOR SIX*

Parameter	Models 1 - 5+					Observed	Model 8				
Concentration ($\mu\text{g}/\text{m}^3$)	1332	2560	1645	1712-2423	671-1139	2077-2971	1760	1384	1963		
Julian day, hour	265,13	265,14	265,15	223,10	223,11	223,12	42,13	42,14	42,15		
SO ₂ emissions (g/s)	7327	7494	7377	5964	5880	5829	6899	6227	6395		
BNA Meteorology											
Wind speed (m/s)	2.1	1.0	2.1	5.1	4.6	5.1					
Flow vector (°)	263	352	342	034	028	036					
Mixing height (m)	1140	1295	1295	1319	1588	1856	1736	2013	2013		
Stability class	B	B	C	C	B	C	C	D	C		
Onsite Meteorology											
110m wind speed (m/s)	2.2	2.1	2.0				2.7	3.2	4.0		
110m flow vector (°)	035	023	035				033	040	038		
ΔT , 110m-10m (K)	-2.1	-2.0	-1.5				-1.7	-1.8	-1.0		
σ_θ , 110m (°)	14	13	15								
σ_ϕ , 110m (°)	16	18	17								

(continued)

TABLE 17. (continued).

Parameter	Model 10			Models 6, 7, and 9**			Model 11		
Concentration ($\mu\text{g}/\text{m}^3$)	3055	1476	1255	1629-1662	1529-3051	1870-3397	2732	2738	2372
Julian day, hour	179,13	179,14	179,15	125,10	125,11	125,12	33,13	33,14	33,15
SO ₂ emissions (g/s)	7018	7080	6998	8302	8585	8988	8528	8044	6879
BNA Meteorology									
Mixing height (m)	1716	1920	1920	1891	1923	1955	1059	1232	1232
Stability class	B	C	D	D	C	B	B	C	C
Onsite Meteorology									
110m wind speed (m/s)	8.5	8.8	7.2	8.1	7.9	6.4	3.0	3.4	3.4
110m flow vector (°)	040	033	032	042	038	037	040	034	041
ΔT , 110m-10m (K)	-1.9	-2.0	-2.0	-1.6	-1.8	-1.7	-2.5	-2.5	-2.2
σ_θ , 110m (°)	6	6	7	8	8	9	10	7	8
σ_ϕ , 110m (°)	6	5	6				9	6	7

*Receptor six is located at an azimuth of 36°.

Data not shown were not used in the modeling.

+Concentrations shown indicate the range of concentrations for the five models.

**Model 9 predicted a concentration of 3051 $\mu\text{g}/\text{m}^3$ for hour 11 and a concentration of 3397 $\mu\text{g}/\text{m}^3$ for hour 12.

Two meteorological alternatives were examined at Johnsonville. The first alternative involved the elimination of calm wind periods from the airport data. The elimination of calm winds, as seen by comparing model 5 to 4 and model 2 to 1, resulted in slightly lower concentrations at three of the eleven receptors. The second meteorological alternative contrasted the use of onsite wind data with airport wind data, as seen by comparing models 4 and 6, respectively. On average, the two models agreed within ten percent although a difference of 40 percent was noted at receptor eight.

Six alternative approaches for dispersion were used at Johnsonville. The models using either PG or Briggs dispersion coefficients, models 6, 7, and 8, agreed within ten percent. The other dispersion schemes, which used onsite turbulence data, showed greater differences. The Pasquill (1976) scheme used in model 9 overpredicted at all but one receptor. The other two dispersion schemes, used in models 10 and 11, yielded both underpredictions and overpredictions, generally within a factor of three to the observations. The Cramer scheme used in model 11 overpredicted the concentration at receptor six by $768 \mu\text{g}/\text{m}^3$ or 42 percent.

The meteorological parameters used in the models and those reported during the observed second-highest 3-hour concentration at receptor six are listed for each hour in Table 17. The meteorological conditions for the observed and modeled concentrations were typified by light winds, limited mixing heights, and unstable conditions. The wind directions used by each model were within six degrees of the

centerline azimuth for receptor six, while the wind directions, reported onsite during the high observed concentrations, were offset by as much as 13° from the receptor azimuth. The airport wind directions were as much as 135° off the centerline azimuth.

Second-highest 24-hour Concentrations

The second-highest observed and predicted 24-hour average SO_2 concentrations at Johnsonville during 1977 are listed in Table 18. The highest second-high concentration, $521 \mu\text{g}/\text{m}^3$, was observed at receptor six. Concentrations exceeding $365 \mu\text{g}/\text{m}^3$ (NAAQS) were also observed at receptor one and receptor seven.

A format similar to that used with the 3-hour analysis was followed. The meteorological conditions concentrations resulting in significant hourly concentrations for receptor six are presented in Table 19.

As seen in Table 18, the differences in concentrations due to different emissions data followed the tendencies noted in the 3-hour analysis. Changing from full-load to hourly emissions reduced the modeled concentrations by an average of 28 percent. The model using hourly emissions data exceeded predictions by the model using daily emissions data by an average of five percent.

The effect of using two meteorological alternatives was also examined. The elimination of calm winds from the airport meteorological data increased concentrations, as much as 19 percent, at eight of the eleven receptors. For the second alternative, onsite versus airport wind data, the model using onsite meteorological data

TABLE 18. SECOND-HIGHEST OBSERVED AND PREDICTED 24-HOUR AVERAGE SO₂ CONCENTRATIONS AT EACH JOHNSONVILLE RECEPTOR DURING 1977*

Receptor	Observed	Model number										
		1	2	3	4	5	6	7	8	9	10	11
1	483 (55)	299 (53)	330 (189)	215 (126)	226 (181)	257 (189)	291 (67)	294 (67)	296 (67)	284 (33)	261 (220)	291 (189)
2	267 (39)	274 (144)	263 (48)	205 (48)	212 (48)	209 (247)	351 (108)	373 (216)	378 (216)	332 (108)	295 (216)	293 (136)
3	168 (343)	321 (47)	350 (47)	220 (322)	241 (156)	263 (156)	214 (82)	220 (282)	226 (82)	259 (82)	258 (282)	268 (152)
4	150 (246)	193 (183)	221 (183)	113 (135)	119 (135)	118 (85)	137 (106)	150 (106)	147 (113)	142 (204)	116 (83)	119 (186)
5	237 (39)	437 (87)	437 (87)	272 (204)	291 (204)	303 (319)	363 (318)	459 (177)	392 (177)	480 (318)	173 (318)	215 (193)
6	521 (117)	385 (159)	396 (189)	282 (181)	299 (181)	334 (189)	495 (178)	518 (67)	517 (178)	574 (52)	501 (125)	487 (52)
7	385 (117)	350 (173)	357 (233)	243 (219)	241 (219)	251 (219)	190 (219)	214 (179)	197 (219)	262 (179)	224 (219)	200 (26)
8	195 (19)	166 (31)	166 (31)	124 (31)	129 (10)	129 (10)	104 (21)	107 (21)	104 (21)	89 (32)	77 (21)	80 (21)
9	209 (16)	234 (282)	241 (36)	188 (343)	196 (289)	196 (289)	285 (316)	288 (316)	342 (275)	349 (36)	275 (36)	212 (47)
10	256 (208)	175 (145)	206 (254)	140 (129)	149 (129)	156 (106)	176 (309)	200 (309)	204 (130)	203 (208)	185 (195)	97 (195)
11	235 (307)	283 (154)	330 (246)	180 (154)	201 (283)	215 (244)	241 (293)	265 (293)	260 (306)	349 (283)	276 (293)	279 (283)

*Numbers in parentheses indicate day of occurrence.
Concentrations are in $\mu\text{g}/\text{m}^3$.

TABLE 19. HOURLY SO₂ CONCENTRATIONS, GREATER THAN 50 µg/m³, AND METEOROLOGICAL PARAMETERS ASSOCIATED WITH THE SECOND-HIGHEST 24-HOUR AVERAGE SO₂ CONCENTRATIONS MODELED AND OBSERVED FOR 1976 AT JOHNSONVILLE RECEPTOR SIX*

Observed (Julian day 117)		522	653	862	1959	967	1620	1855	1306	914	52	888	52	78	340	157	346	104	131
Concentration (µg/m ³)	Hour (local time)	01	02	03	04	05	06	07	08	09	10	11	15	16	17	18	19	20	21
SO ₂ emissions (g/s)		7849	7871	7865	7875	7735	7865	7793	8002	8120	8065	8088	7868	7838	7945	7699	7930	7877	7915
BNA Meteorology																			
Wind speed (m/s)		3.1	4.1	3.6	4.1	4.6	5.7	4.6	7.2	5.7	5.1	5.7	5.1	5.1	6.7	4.6	4.1	4.1	3.6
Flow vector (°)		009	020	009	020	017	091	069	077	095	090	092	090	078	068	064	046	039	006
Mixing height (m)		-	-	-	-	-	353	729	1105	1482	1858	2234	3363	3363	3363	3363	-	-	-
Stability class		F	E	E	E	E	D	C	D	C	C	C	C	D	D	D	E	E	E
Onsite Meteorology																			
110m wind speed (m/s)		7.1	7.1	7.7	-2	5.5	6.2	5.8	5.5	4.5	4.7	5.4	7.5	7.6	8.4	8.2	7.6	6.6	8.0
110m flow vector (°)		350	343	344	352	359	355	350	343	050	066	M	M	M	M	M	M	M	M
ΔT, 110m-10m (K)		+5.1	+3.5	+4.2	+1.6	+1.4	+0.9	+0.5	-0.4	-1.4	-1.7	-2.2	-2.5	-2.0	-1.7	-1.6	-0.4	+0.9	+2.3
Q ₀ , 110m (°)		4	5	5	5	7	7	7	9	11	11	M	M	M	M	M	M	M	M
Q ₀ , 110m (°)		3	3	3	3	6	5	5	6	8	9	M	M	M	M	M	M	M	M
Model 1 (Julian day 159)																			
Concentration (µg/m ³)	Hour (local time)	09	11	12	19	20	21	22	23	24									
BNA Meteorology																			
Wind speed (m/s)		4.6	6.2	5.7	5.7	4.1	5.1	5.1	6.7	5.7									
Flow vector (°)		047	040	036	043	038	039	040	039	037									
Mixing height (m)		1065	1545	1785	2265	-	-	-	2160	2134									
Stability class		C	C	C	D	E	E	E	D	D									

continued

TABLE 19. (continued)

Model 7 (Julian day 67)											
Concentration ($\mu\text{g}/\text{m}^3$)	170	268	87	1248	1147	1614	1549	1170	1861	1784	1439
Hour (local time)	04	05	07	08	10	11	12	13	14	15	16
SO ₂ emissions (g/s)	10500	10518	11501	11616	10564	9868	7838	7330	7110	7139	7701
BNA mixing height (m)	-	-	E	-	519	1102	C	D	D	D	D
BNA stability class	F	G	-	D	C	C	C	D	D	D	D
110m wind speed (m/s)	6.4	5.8	5.0	5.7	3.4	3.3	5.3	7.1	7.8	6.5	7.1
110m flow vector (°)	036	037	035	037	033	045	041	032	037	036	042
Model 9 and Model 11 (Julian day 52)											
Concentration ($\mu\text{g}/\text{m}^3$)	2827	1965	3647	4773							
Model 11	2628	2201	3010	3368							
Hour (local time)	11	12	13	14							
SO ₂ emissions (g/s)	8244	8063	8109	8101							
BNA mixing height (m)	1331	1630	1929	2228							
BNA stability class	B	C	B	B							
110m wind speed (m/s)	2.4	3.5	3.6	3.8							
110m flow vector (°)	035	033	035	037							
ΔT , 110m-10m (K)	-2.5	-2.7	-2.8	-2.7							
σ_0 , 110m (°)	10	7	7	7							
σ_0 , 110m (°)	12	8	8	8							
Model 10 (Julian day 125)											
Concentration ($\mu\text{g}/\text{m}^3$)	71	1360	2185	2691	3306	492	1877				
Hour (local time)	08	10	11	12	13	14	15				
SO ₂ emissions (g/s)	7794	8302	8585	8988	9206	9302	9449				
BNA mixing height (m)	1828	1891	1923	1955	1986	2018	2018				
BNA stability class	C	D	C	B	C	D	C				
110m wind speed (m/s)	8.9	8.1	7.9	6.4	6.8	6.8	6.7				
110m flow vector (°)	024	042	038	037	053	029	032				
ΔT , 110m-10m (K)	-0.3	-1.2	-1.3	-1.3	-1.3	-1.3	-1.4				
σ_0 , 110m (°)	8	8	8	9	7	7	8				
σ_0 , 110m (°)	15	14	14	13	6	6	8				

*Receptor six is located at an azimuth of 36°.

Only hourly concentrations above $50 \mu\text{g}/\text{m}^3$ are reported above.

Parameters listed for the modeling results are those used in the model input.

M = missing data

exceeded predictions of the model using airport meteorological data by about ten percent. Differences between the two models at each receptor ranged from -21 to +50 percent.

The results of the models using different dispersion schemes also followed a pattern similar to that for the 3-hour average analysis. The models using buoyancy-induced-dispersion, models 7 and 8, showed an average increase of ten percent over the model using the PG dispersion coefficients. The model using Pasquill's (1976) recommendation resulted in an average increase of 20 percent over the PG model. On average, the models using the two turbulence schemes, models 10 and 11, were within ten percent of the PG model. However, rather substantial overpredictions were noted at receptor three and substantial underpredictions were noted at receptor ten.

The conditions resulting in the second-highest 24-hour average concentrations are given in Table 19. The conditions associated with the observations and each group of models are described below. The second-highest observed concentration was reported for day 117. This day was characterized by various meteorological conditions, with stability classes from BNA ranging from C to F. Wind speeds from the 110 m onsite tower averaged 7 m/s. Unfortunately, turbulence data and wind directions were missing for 13 of the 24 hours during day 117.

For model 1, the second-highest 24-hour average concentration at receptor six was predicted for day 159. Concentrations exceeding 100 $\mu\text{g}/\text{m}^3$ were predicted for 9 of the 24 hours with model 1 on day 159. Stability classes used in model 1 ranged from C to E. For the 9 hours with high concentrations, wind speeds were moderate and flow vectors were within five degrees of the azimuth centered on receptor six.

For models 2 and 5, the second-highest 24-hour concentration was predicted for day 189. During day 189, only four hours of data resulted in predicted concentrations that were greater than $100 \mu\text{g}/\text{m}^3$. The meteorology for these four hours was characterized by unstable conditions, stability classes B and C, and low mixing heights. The estimated hourly emissions were lower than average.

For models 3 and 4, the second-highest 24-hour average concentration was predicted for day 181. Five hours of data yielded concentrations that exceeded $100 \mu\text{g}/\text{m}^3$. The meteorology for these hours was characterized by moderate winds and stability class C or D. Also, the flow vectors were directed, during these five hours, within a ten degree sector centered towards receptor six.

With models 6 and 8, the second-highest concentration was predicted to occur for day 178. Concentrations exceeding $100 \mu\text{g}/\text{m}^3$ were predicted with 9 of the 24 hours of data. These nine hours exhibited stabilities that ranged from B to E. Wind speeds were moderate, during these hours, and the flow vectors were within ten degrees of the centerline azimuth.

Model 7 predicted the second-highest 24-hour concentration for day 67. Ten hours of data on day 67 resulted in concentrations that were greater than $100 \mu\text{g}/\text{m}^3$.

The models using onsite turbulence data, models 9 and 11, predicted that the second-highest 24-hour concentration would occur on day 52. For both models, predictions greater than $2000 \mu\text{g}/\text{m}^3$ were noted on four separate hours. The meteorological data used in the models on these hours were characterized by unstable conditions (stability classes B and C) and light, persistent winds.

The other model using onsite turbulence data, model 10, predicted that the second-highest 24-hour concentration would occur on day 125. Concentrations exceeding $100 \mu\text{g}/\text{m}^3$ were predicted for this day on 6 of the 24 hours. The meteorology during these hours was characterized by stability classes ranging from B to D and by moderate wind speeds.

Geometric Mean Concentrations

Geometric mean concentrations were computed from the top 25 1-hour, 3-hour, and 24-hour average concentrations predicted by the 11 models and observed at Johnsonville during 1977. Receptor eight was not included in this calculation because of poor data recovery. A comparison of the observations and each model is shown in Figures 25-35. A descriptive summary of this comparison is given in Table 20.

DIAGNOSTIC EVALUATION

Pollution Roses

Pollution roses were plotted for each receptor from the top 25 hourly concentrations observed at each receptor. As shown in Figure 36, the pollution roses reflect that the wind directions measured onsite were as much as 180° off the azimuth directed from the power plant to the receptor during high measured concentrations. In contrast, modeled concentrations for each of the 11 models were associated with wind directions that were within a ten degree azimuth centered on each receptor during the top 25 hourly concentrations.

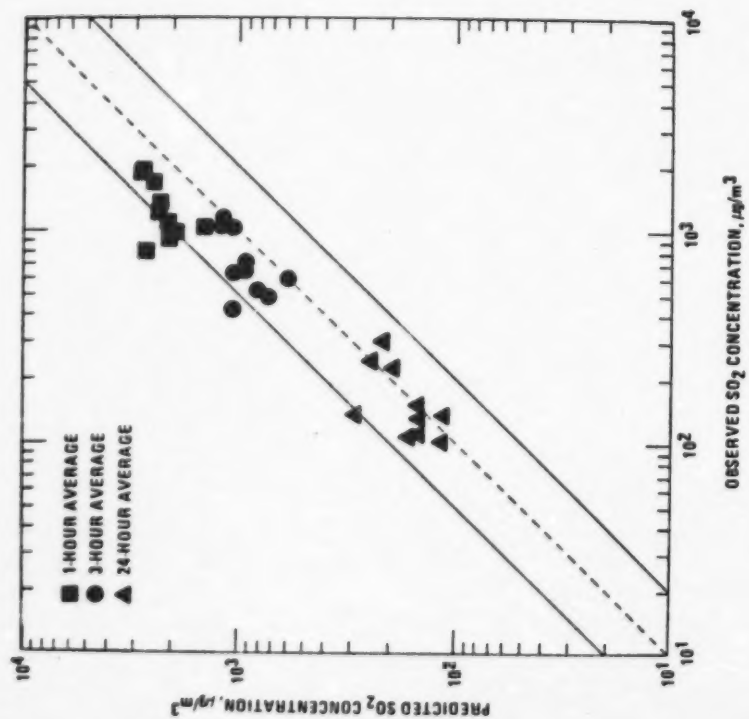


Figure 25. Comparison of model 1 and observed geometric means of the top 25 1-, 3-, and 24-hour average concentrations at Johnsonville, TN, during 1977.

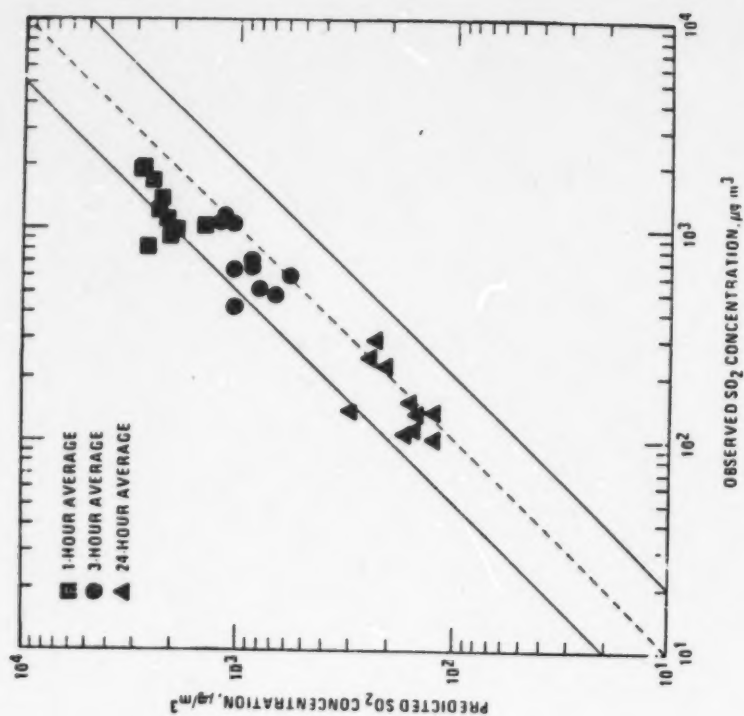


Figure 26. Same as Figure 25, except for model 2.

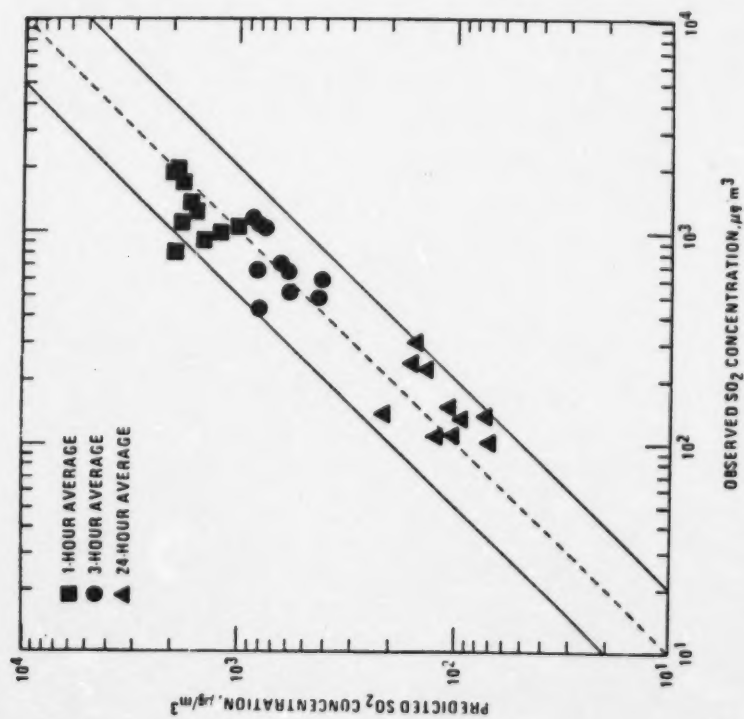


Figure 27. Same as Figure 25, except for model 3.

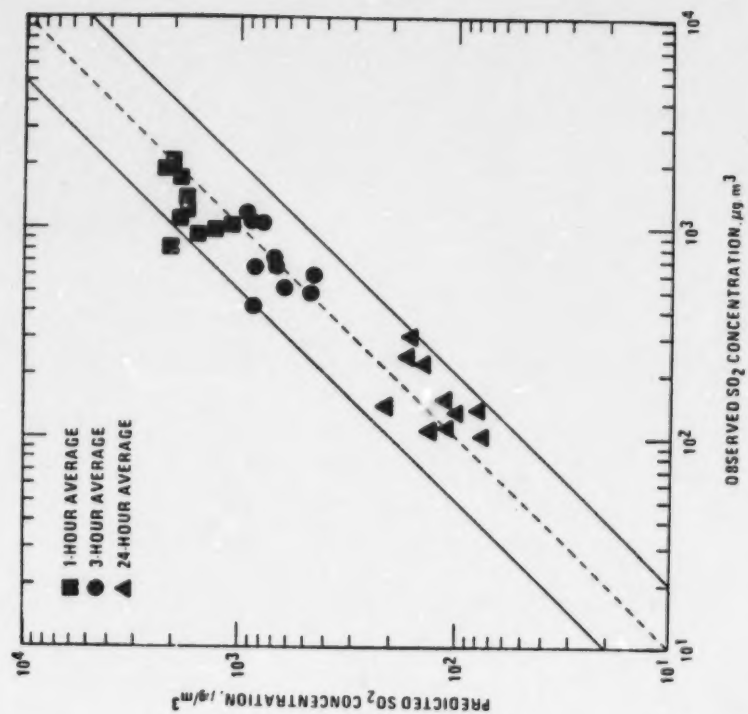


Figure 28. Same as Figure 25, except for model 4.

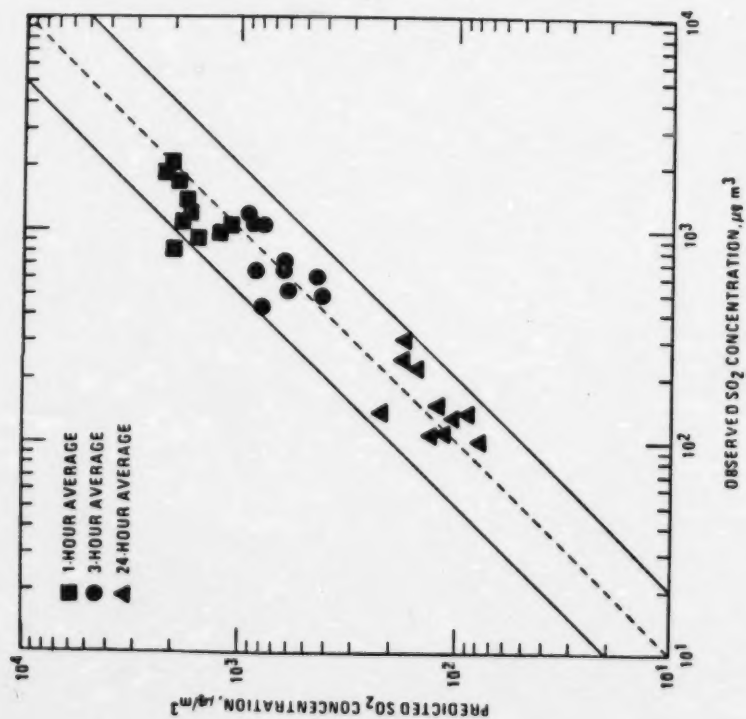


Figure 29. Same as Figure 25, except for model 5.

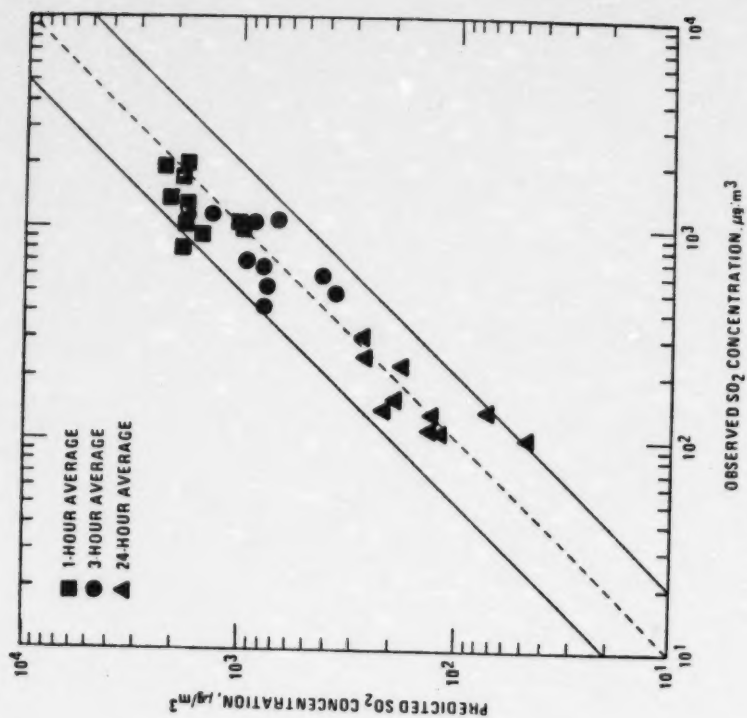


Figure 30. Same as Figure 25, except for model 6.

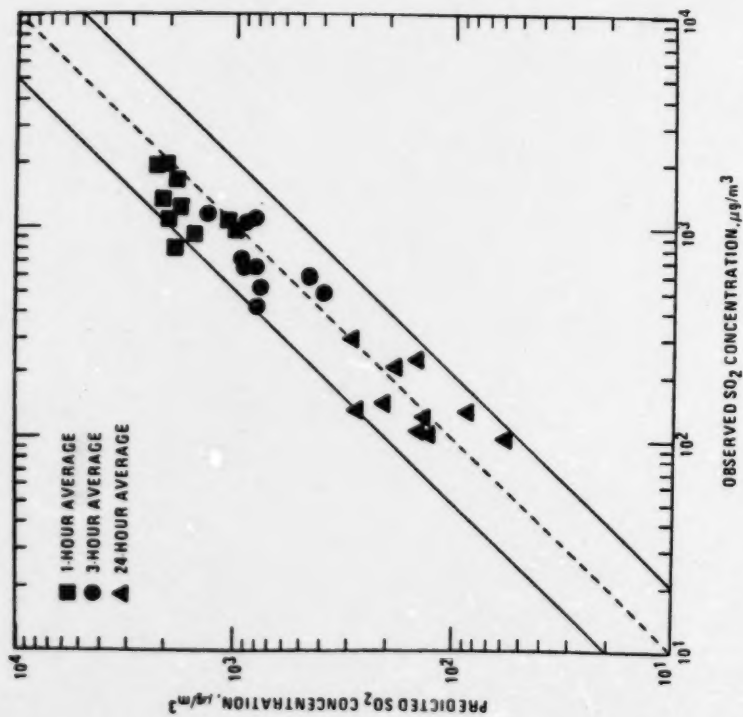


Figure 31. Same as Figure 25, except for model 7.

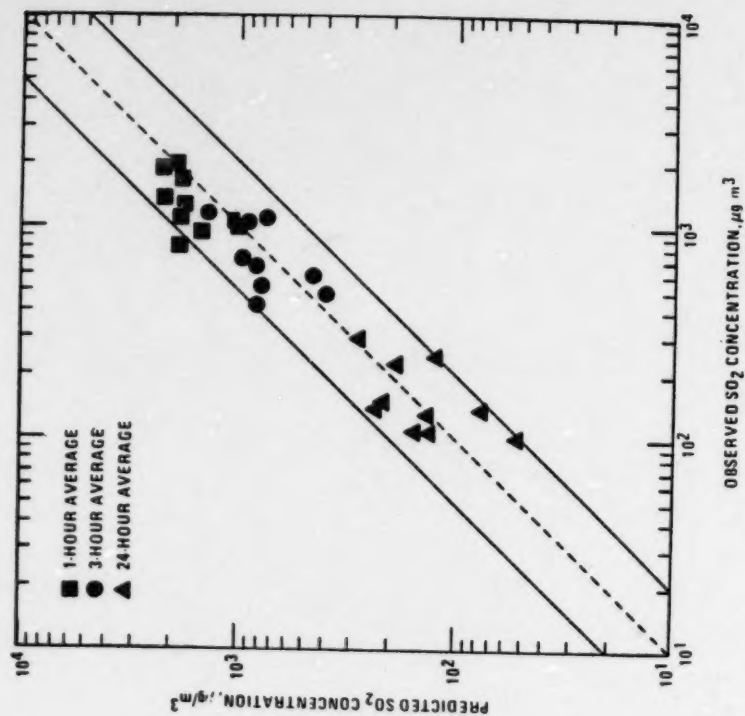


Figure 32. Same as Figure 25, except for model 8.

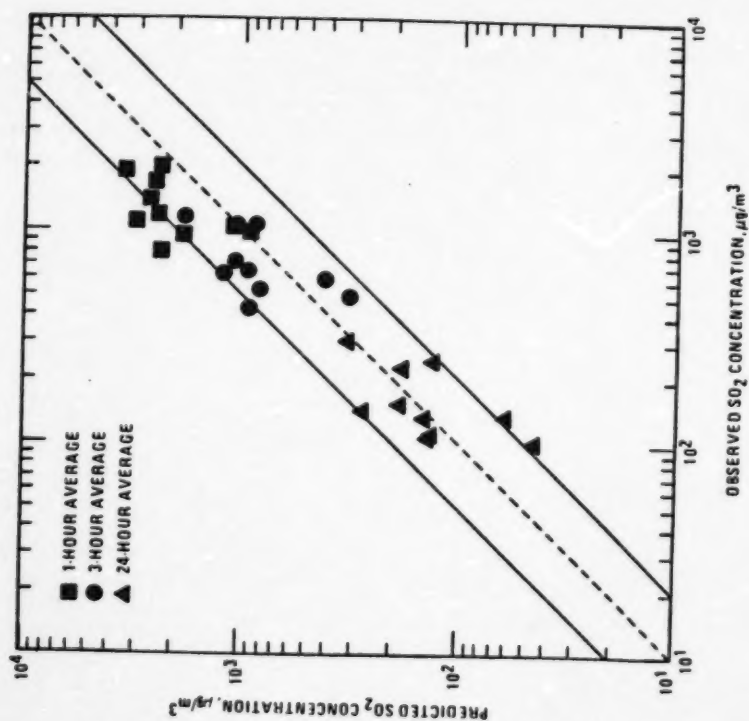


Figure 33. Same as Figure 25, except for model 9.

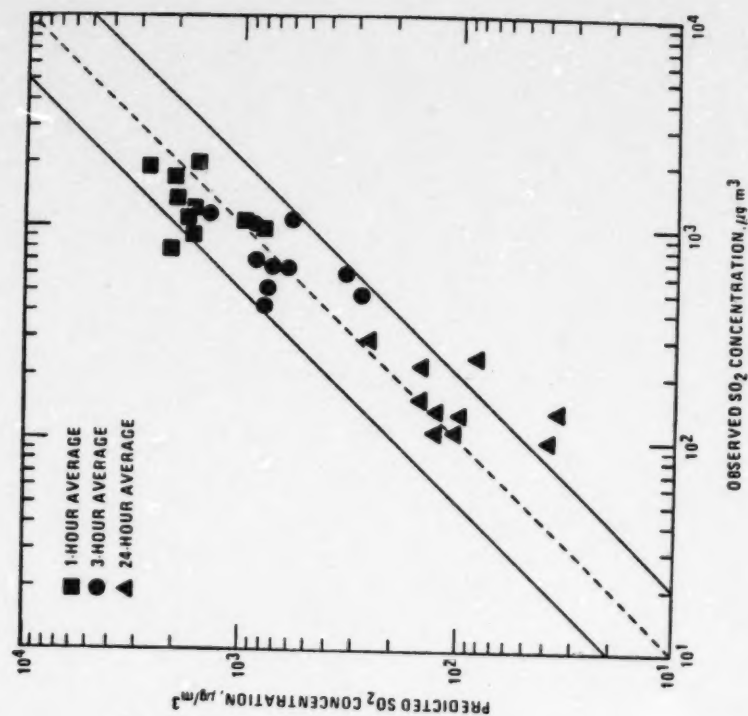


Figure 34. Same as Figure 25, except for model 10.

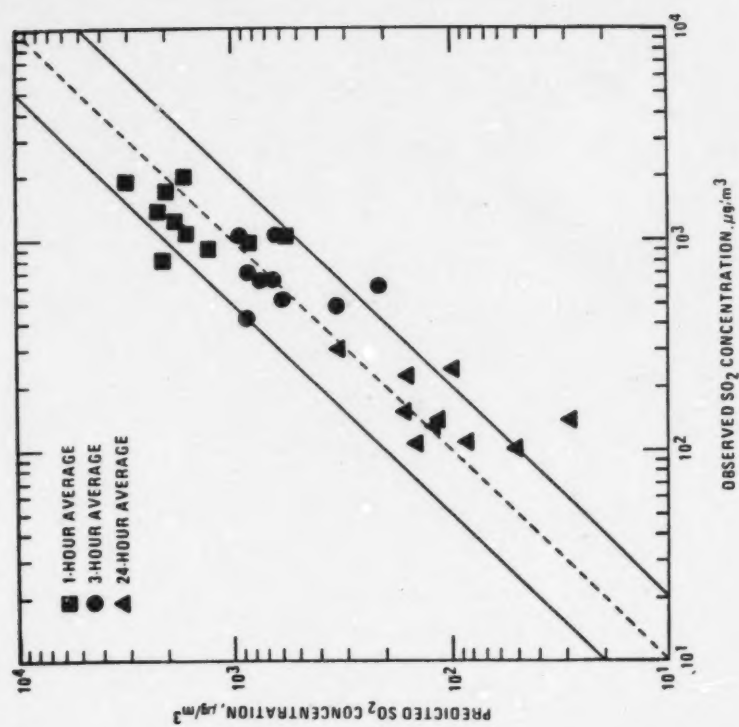


Figure 35. Same as Figure 25, except for model 11.

TABLE 20. DESCRIPTIVE SUMMARY OF THE GEOMETRIC MEANS COMPUTED FOR THE TOP 25 1-HOUR, 3-HOUR, AND 24-HOUR AVERAGE SO₂ CONCENTRATIONS MODELED FOR JOHNSONVILLE FOR 1977

Model	Percent of geometric means greater than a factor of 2	Percent of geometric means less than a factor of $\frac{1}{2}$	Remarks
1	16.7	0.0	1-hour and 3-hour concentrations were overpredicted at every receptor; tended to overpredict overall
2	16.7	0.0	almost identical to model 1
3	3.3	0.0	tended to overpredict for the longer averaging times
4	3.3	0.0	similar to model 3
5	3.3	0.0	similar to model 3
6	3.3	3.3	tended to overpredict 1-hour concentrations
7	3.3	0.0	1-hour concentrations were overpredicted, but 24-hour concentrations were predicted better than with model 6
8	3.3	0.0	24-hour predictions reduced slightly compared with model 7
9	10.0	6.7	most 1-hour and 3-hour concentrations were overpredicted
10	3.3	10.0	1-hour concentrations were overpredicted, 3-hour predictions compared favorably, 24-hour concentrations were overpredicted
11	6.7	10.0	much scatter with underpredictions and overpredictions, tended to underpredict 24-hour concentrations

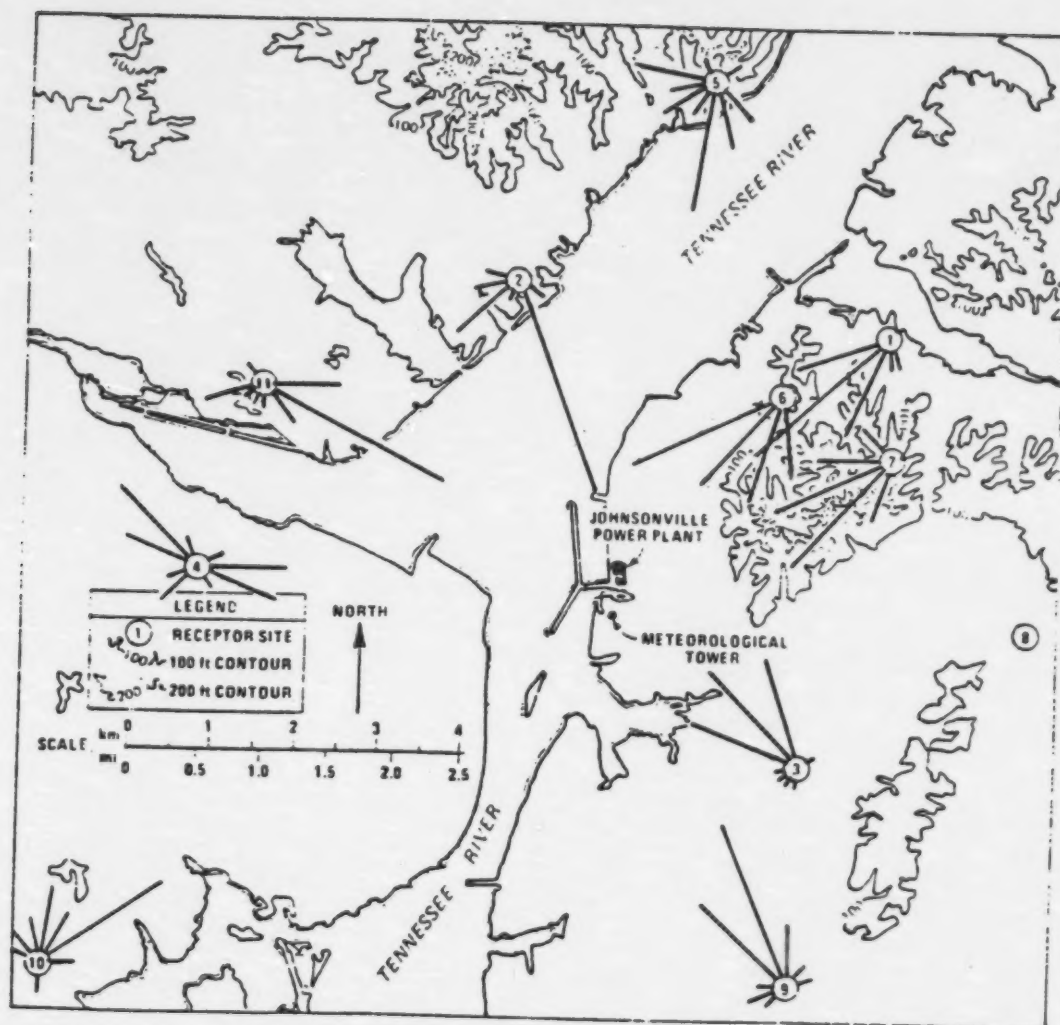


Figure 36. Pollution roses of the top 25 hourly SO_2 concentrations (observed at each receptor) at Johnsonville using 110 m wind direction data from the onsite meteorological tower.

Pearson Correlation Coefficients

Pearson correlation coefficients were computed from each valid hour of paired observed and modeled concentration during 1977. The computed coefficients are listed in Table 21. For each model and receptor, the correlation coefficients were significantly greater than the zero correlation at a significance level of 99 percent. As with the Paradise results, these coefficients remained quite low.

Meteorological Stratification

The hourly concentration data for Johnsonville were stratified for selected models and selected receptors by stability class. The procedure used to stratify the data differed slightly from the Paradise analysis, as noted below:

- 1) Four receptors representing a range of distances and terrain heights were selected: receptor 5 (6.55 km, $\Delta h = 47$ m), receptor 6 (3.27 km, $\Delta h = 43$ m), receptor 9 (5.71 km, $\Delta h = 1.5$ m), and receptor 10 (8.66 km, $\Delta h = 10.7$ m).
- 2) Seven models representing significant differences in modeling procedures were selected, models 1, 3, 6, 8, 10, and 11.
- 3) The data were analyzed only when the 110 m onsite wind vector was reported for a $22\frac{1}{2}^\circ$ sector directed towards the receptor.

The mean fraction error (MFE) was again used as the statistic for this analysis, where a value of 66.67 percent denoted an error of a factor of two. The MFEs were computed for stability classes B, C, D, and E. Not enough data were available for A-stability to warrant its inclusion into the analysis. The MFEs were plotted as function of stability for each receptor, as shown in Figures 37-40.

TABLE 21. PEARSON CORRELATION COEFFICIENTS COMPUTED FROM VALID HOURLY PREDICTED AND OBSERVED SO₂ CONCENTRATIONS AT JOHNSONVILLE DURING 1977

Receptor	Model										
	1	2	3	4	5	6	7	8	9	10	11
1	.12	.12	.13	.12	.12	.26	.27	.29	.20	.21	.24
2	.09	.09	.09	.09	.09	.11	.12	.13	.10	.08	.08
3	.10	.10	.11	.10	.10	.21	.23	.24	.23	.23	.31
4	.09	.09	.09	.09	.10	.21	.21	.22	.18	.20	.19
5	.10	.10	.09	.09	.10	.15	.14	.16	.10	.08	.07
6	.14	.13	.14	.14	.14	.28	.30	.30	.24	.23	.28
7	.11	.11	.11	.11	.11	.24	.27	.27	.20	.18	.24
9	.24	.22	.23	.24	.23	.30	.31	.31	.29	.30	.31
10	.12	.13	.13	.12	.12	.20	.21	.21	.16	.15	.17
11	.16	.16	.17	.18	.17	.28	.31	.30	.25	.33	.30

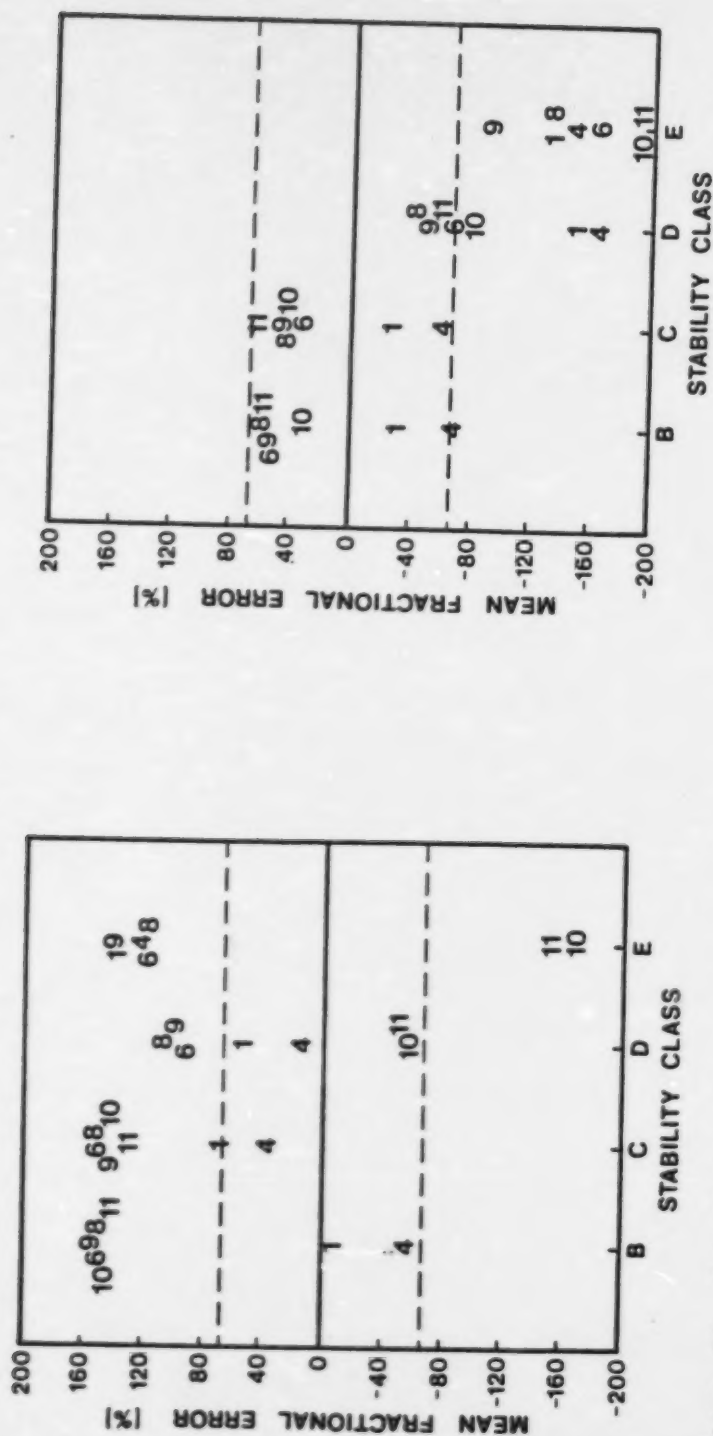


Figure 37. Mean fractional errors computed for each alternative model (numbered from 1 to 11) and stratified by stability class at Johnsonville receptor five ($x = 6.6$ km).

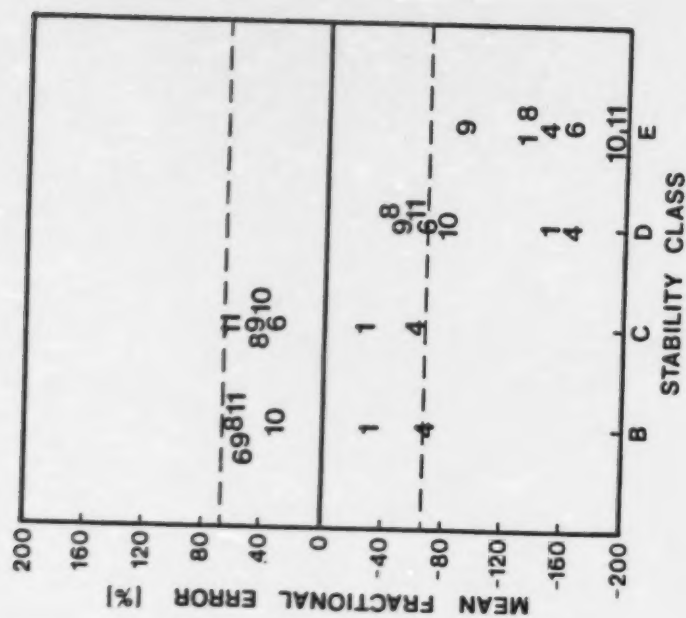


Figure 38. Same as Figure 37, except for receptor six ($x = 3.3$ km).

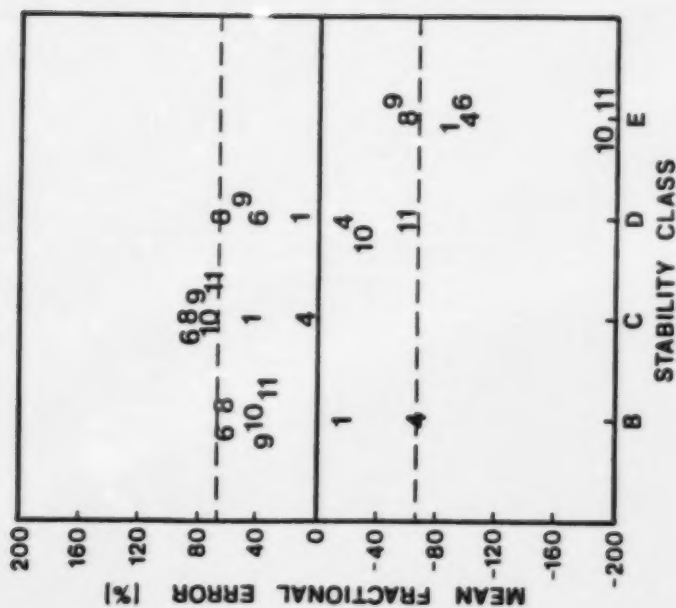


Figure 39. Same as Figure 37, except for receptor nine ($x = 5.7$ km).

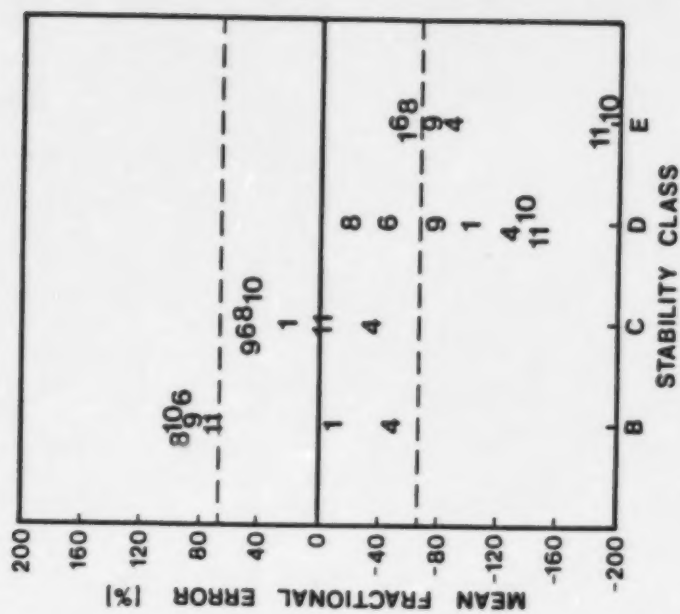


Figure 40. Same as Figure 37, except for receptor ten ($x = 8.7$ km).

SECTION 8

JOHNSONVILLE DISCUSSION

The modeled and observed SO₂ concentrations for the Johnsonville plant during 1977 were examined. Although a limited number of statistical tests were performed, these tests hopefully highlighted some of the important differences in the modeling alternatives. This section is divided into a discussion of peak concentrations and diagnostic evaluation.

PEAK CONCENTRATIONS

This section considers the results from the second-highest 3-hour and 24-hour average concentrations, and the analysis of the top 25 geometric mean concentrations. This discussion is further divided into three major modeling categories: emissions, meteorology, and dispersion.

Emissions

The differences in peak concentrations attributable to alternative SO₂ emission rates and stack operating parameters were evaluated by comparing a model that used emission parameters associated with 100 percent design-load characteristics against models that used hourly and daily average emission parameters. As expected, the second-highest 3-hour and 24-hour average concentrations were reduced by 3 to 40 percent when hourly and daily stack characteristics were used instead of full-load characteristics. The differences in

concentrations between the models using hourly and daily average emissions data, however, differed by less than five percent. This result seems reasonable because the mean emission rates for the daily and hourly parameters varied by only 6 percent.

The geometric mean concentration analysis showed that the models using full-load characteristics tended to overpredict, while the models using hourly and daily emissions data tended to underpredict. Nevertheless, both model alternatives were generally within a factor of two of the observations.

The listing of the meteorological conditions, associated with the second-highest 3-hour and 24-hour concentrations at receptor six, showed that the conditions producing peak concentrations were similar for all three emission models. For this 3-hour period, the concentrations predicted by the models using hourly and daily emissions data were, on average, 20 percent lower than the concentrations predicted by the full-load emissions model. Yet, the actual SO_2 emission rates used by the daily and hourly models were about 45 percent lower than the emission rates used in the full-load emissions model. This suggests that the reduction in stack exit velocities and stack gas temperatures associated with the lower load conditions served to decrease plume rise and resulted in increased ground-level concentrations near the plant.

Meteorology

Elimination of Calm Winds

The predictions of the second-highest 3-hour and 24-hour concentrations showed mixed results when the calm wind periods were eliminated in the input data. The 3-hour concentrations decreased on average by four percent; the 24-hour concentrations, in contrast, showed a net increase of eight percent. The increased concentrations for the 24-hour predictions did improve comparisons at the receptors having the highest observed concentrations - receptors one, six, and seven. The probable reason for the higher 24-hour concentrations is that the calm wind conditions did not result in significant ground-level concentrations, either predicted or observed, at the Johnsonville site. In fact, Tables 17 and 19 showed that moderate wind speeds were associated with the high concentration periods. Therefore, because the 24-hour periods were shortened by each hour of calm winds, the remaining hours of moderate winds contributed to an increase in the average 24-hour concentration. The 3-hour concentration could not have been increased, because the entire 3-hour period was eliminated from the analysis whenever a calm wind was reported.

The elimination of calm winds produced little change in the analysis of the top 25 geometric mean concentrations. Again, this was probably the result of the moderate wind speeds having the greatest influence on high surface concentrations.

Onsite versus Airport Wind Data

The differences between using BNA airport wind data and onsite wind data were evaluated. Because meteorological data from NWS stations are often easily obtained, they are frequently used in EPA regulatory modeling activities. The use of onsite meteorological data, however, has been strongly encouraged by the EPA (1978) and by the AMS (1981b). For this analysis, the onsite wind speeds and wind directions were used for comparison to the airport wind data. The stability class and mixing height information from BNA were incorporated into the onsite meteorological data base.

The model using onsite wind data produced higher concentrations at nine of the eleven receptors for the 3-hour and 24-hour concentrations. The average increase in concentrations for the model using onsite wind data relative to the model using airport wind data was three percent for the 3-hour concentrations and 15 percent for the 24-hour average concentrations. The geometric mean concentrations, however, for both models were in good agreement to the observations.

The primary difference between the two modeling alternatives was the wind speed. In the final data set, the wind speed from the airport averaged 1.4 m/s greater than the 110 m onsite wind speed. Note that the wind speeds for the BNA data were extrapolated to the 110 m height using power-law exponents for each stability class. The increased dilution associated with higher wind speeds could account for the lower concentrations from the airport data. However, the effects of reduced plume rise, not addressed in this study, need to be understood in order to fully assess the effects of increased wind speed.

Dispersion

Similar results were noted with the models using the three basic dispersion schemes: PG, PG with buoyancy-induced-dispersion (BID), and Briggs with BID. In predicting the second-highest 3-hour concentration, the models using BID produced slightly higher concentrations than the model using PG coefficients at seven of the eleven receptors. Furthermore, a net increase of ten percent was noted in the second-highest 24-hour concentrations predicted by the models using BID. Nevertheless, these models resulted in significant underpredictions of the peak concentrations at the receptors reporting the highest observed concentrations: receptors one, six, and seven. The higher predictions from the models using BID were also noted in the analysis of geometric mean concentrations, especially for the 24-hour averaging time. However, 90 percent of the geometric mean predictions for the three models were within a factor of two of the geometric mean observations. The relatively small increase in predicted concentrations found with BID probably occurred because the receptors at Johnsonville were situated more than 2 km from the plant complex. Sensitivity studies by Turner (personal communication, 1981) have shown that the greatest effect in ground-level concentrations due to BID will occur at distances within 1 km of an elevated source. The differences between the model using Briggs coefficients and the model using PG coefficients were minimized because the peak concentrations at Johnsonville were associated with B and C stabilities. The greatest differences between these two schemes is expected with A-stability.

The model based on Pasquill's (1976) recommendation produced higher peak concentrations than the models using any other dispersion scheme. In comparison to the PG model, the second-highest 3-hour concentrations predicted by the Pasquill (1976) model were, on average, 39 percent higher than the PG model; second-highest 24-hour concentrations were 20 percent higher. In addition, the geometric mean concentrations were overpredicted at most receptors, and ten percent of the receptors were overpredicted by more than a factor of two. This tendency for Pasquill's approach to overpredict may be due to the combined use of different meteorological data bases. In this study, σ_z was determined from the BNA stability class, and σ_y was determined from onsite σ_θ measurements. As shown in Tables 17 and 19, the peak concentrations from the Pasquill approach occurred when large σ_z and small σ_y values were used in the model.

The results from the models using the other onsite turbulence schemes showed mixed results. On average, the Draxler and the Cramer approaches agreed within ten percent of the PG model on predictions of the second-highest 3-hour and 24-hour concentrations. Both overpredictions and underpredictions were noted for the 3-hour concentrations. At receptor six, an overprediction of $83 \mu\text{g}/\text{m}^3$ was noted with the Draxler model, and an overprediction of $765 \mu\text{g}/\text{m}^3$ was noted with the Cramer model. The peak 24-hour concentrations, however, were underpredicted by an average of five percent and ten percent with the Draxler and Cramer models, respectively.

Underpredictions for the 24-hour concentrations seemed to be the result of limiting the growth of σ_z in the nighttime hours. As the observations showed, high concentrations were reported at night during neutral and slightly stable conditions.

The geometric mean concentration analysis indicated varied results from the two models. The 3-hour geometric mean concentrations agreed fairly well with the observed concentrations. However, the 1-hour concentrations were overpredicted by both models, and the 24-hour concentrations were underpredicted.

DIAGNOSTIC EVALUATION

This section discusses the evaluation of model performance by using a limited set of statistics. First, this evaluation includes the computation of Pearson correlation coefficients for each valid hour of paired modeled and observed concentrations at each receptor. It also includes the computation of average model bias as a function of stability for selected receptors and models.

Pearson Correlation Coefficients

The Pearson correlation coefficients computed from Johnsonville demonstrated, like those computed for the Paradise plant, that predictions from even more sophisticated models did not compare favorably with observations on an hour-by-hour basis. The highest correlation coefficient computed with the Johnsonville data was 0.31. However, all correlation coefficients were statistically significant; that is, the null hypothesis of no correlation could be rejected.

Correlations computed for the model using onsite wind data were higher than those computed for the models using the airport data. This suggests that meteorological data played an important role in improving comparisons of hourly observations to model predictions.

Mean Fractional Errors

The final statistic used with the Johnsonville data was the mean fractional error (MFE). The MFE is simply used to indicate the average model bias as a function of stability class. It does not reveal the hour-by-hour dissimilarities between the predictions and the observations. This statistic seems to be appropriate for use because errors in wind direction tend to obscure the overall trends in modeling results. Thus, four receptors and seven models were selected for evaluation.

The effects of emission rates and stack parameters were noted by comparing the models using full-load emissions data against the models using hourly emissions data. As expected, the models using hourly emissions data showed lower concentrations relative to the models using full-load emissions data. Furthermore, the models using the emissions data underpredicted the average concentrations for all stabilities at all four receptors. The model using full-load emissions data produced mean concentrations that were within a factor of two for the B and C-stability groupings. The lower MFE calculated for the model using hourly emissions data was roughly proportional to the reduced emission rates, as compared to the full-load emission rates.

Rather significant differences were apparent between the model using airport meteorological data and the model using onsite wind data, models 4 and 6 respectively. The model using airport data underpredicted the concentrations at all four receptors while the other model yielded higher MFEs. The difference in MFE values further reflects the sensitivity of the Gaussian models to wind direction. With the screening criteria used in this study, only the concentrations for those hours when the onsite 110 m winds blew in a $22\frac{1}{2}^\circ$ sector centered towards the receptor were selected. Consequently, the MFE analysis suggests that the wind directions from the airport data were directed off centerline and resulted in lower concentrations. Furthermore, the difference between the MFEs for the two models was more pronounced for the B-stability grouping. This implies that the lighter wind speeds associated with B-stability, as compared to C and D-stability, were less representative of the wind directions affecting plume transport at the Johnsonville site.

The differences between the models using the various dispersion schemes were not generally as extreme as those noted for the emissions and meteorological alternatives. For stability classes B and C, the MFEs for the models using the five dispersion schemes were within 20 percent. As expected, the MFEs for the models using onsite turbulence data declined during stability classes D and E. This decline was due to the assumption used in the dispersion algorithm that σ_z would effectively equal zero during nighttime hours. This assumption consequently resulted in near zero ground-level concentrations. The

overpredictions noted in the peak concentration analysis with the model using Pasquill's (1976) recommendations did not show up in the MFE analysis. In the peak concentration analysis, the concentrations were apparently caused by the small σ_θ values and the large σ_ϕ values. It is believed, however, that by including the cases of large σ_θ values and small σ_ϕ values into the MFE analysis that the MFE values for this model averaged out to more reasonable values. The effect of buoyancy-induced-dispersion in the models increased concentrations, as reflected in the higher MFE values.

Like Paradise, the models tended to underpredict with increasing stability. However, this tendency was not as well-defined at Johnsonville. The scatter in the MFE values between receptor sites could be due to terrain effects. Although it was initially believed that the terrain effects were insignificant around the Johnsonville plant, two receptors used in the MFE analysis were located 40 m above plant grade or about one-third of the stack height. The effect of using terrain adjustment coefficients, therefore, cannot be ignored. In the modeling, full adjustment was applied to plume height relative to terrain for stability classes A to D. For stability classes E and F, the plume was kept at the same height relative to sea level. The terrain adjustment then may have hindered understanding of the model differences as a function of stability class. But, at receptors five and six, the terrain adjustment did not seem to have caused a higher MFE value as compared to the "flat-land" receptors nine and ten.

SECTION 9

SUMMARY AND RECOMMENDATIONS

EPA routinely uses Gaussian plume models to make decisions having important environmental and economic impacts on air quality. However, as pointed out in the literature survey, further validations and improvements are needed for these models. This study has strived to contribute towards this endeavor.

This study included an evaluation of a Gaussian plume dispersion model with alternative techniques using a rather comprehensive data base developed for two TVA coal-fired power plants, Johnsonville and Paradise. Short-term SO_2 concentrations were evaluated at Paradise with seven modeling alternatives and at Johnsonville with eleven modeling alternatives. The accomplishments of this study included the following:

- 1) The development of two years of data (one year for Paradise and one year for Johnsonville) consisting of hourly SO_2 emission rates and stack characteristics, hourly SO_2 concentrations monitored at ten to twelve receptor sites, hourly average onsite meteorological parameters, and hourly National Weather Service (NWS) meteorological data collected at Nashville, Tennessee (BNA), and Evansville, Indiana (EVV);
- 2) The incorporation of alternative modeling techniques into the EPA Gaussian plume dispersion model, MPTEP, including modifications of MPTEP to allow for the input of onsite meteorological

data, the development of an algorithm for calculating dispersion using Briggs' rural interpolation formulae, and adaptations of onsite turbulence schemes using methods described by Pasquill (1976), Draxler (1976), and Cramer (1976);

3) The implementation of these models using the available data on EPA's UNIVAC computer; and

4) The analysis of the models' results and observed SO_2 concentrations by using relatively straightforward statistical comparisons.

PARADISE

At the Paradise plant, greater differences in predicted SO_2 concentrations resulted from using various emissions data than from using alternative dispersion schemes and meteorological data. Furthermore, the "conservative" full-load emissions models compared more favorably to peak observed concentrations than the "more realistic" models using hourly emissions data, which underpredicted peak concentrations by about a factor of two. This unexpected result was attributed to inaccuracies associated with estimating stability, mixing heights, wind vectors, and/or SO_2 emission rates.

Another unexpected feature of the Paradise analysis was that the models incorporating onsite wind data did not show significant improvements over the models using airport meteorological data.

Although the concentrations from the two modeling alternatives differed hour-to-hour, the overall results, especially for the peak concentrations, were similar. The hour-to-hour differences in concentrations were attributed to the wind flow vectors used to simulate the location of the plume centerline. Yet even with more representative 110 m wind data, the plume trajectories were not depicted with enough accuracy to significantly improve hourly predictions. Therefore, it appears that more accurate procedures for determining plume trajectories are needed so that other important meteorological parameters, such as stability class, can be assessed.

Although emissions input and meteorological data have been recognized as having important effects in dispersion modeling (Fox, 1981), dispersion schemes are usually discussed in greater detail (AMS, 1981b). The concentrations predicted with the three dispersion schemes at Paradise, however, resulted in average differences of less than ten percent. Buoyancy-induced-dispersion did seem to increase concentrations with the models using the Briggs and PG dispersion coefficients, although the Briggs coefficients potentially can yield lower concentrations for downwind distances up to two kilometers. Further measurements taken from receptors closer to the source than those located at Paradise should be examined for comparison between the Briggs and PG curves.

JOHNSONVILLE

With the eleven Johnsonville alternative models, the principal emphasis was on the prediction of peak concentrations, especially the concentrations related to the NAAQS for SO_2 . Some additional analyses were used to diagnostically evaluate the models.

The significant differences between the emissions data alternatives that were noted in the Paradise analysis were not evident in the Johnsonville analysis. In fact, the models using full-load emissions data compared similarly to the models using hourly and daily emissions data for the peak concentrations. The differences between the models using daily and hourly emissions data seemed insignificant; in retrospect, it probably would have been more cost-effective to use the daily emission rates rather than the hourly emission rates. The similar performance noted for the models using full-load, daily, and hourly emission rates may be due to the increased plume rise associated with full-load stack parameters, which in turn caused a reduction in maximum surface concentrations.

The AMS (1981) recently presented reviewers' recommendations that asked for calm winds to be treated differently in the EPA guideline models, including MPTER. One of the models evaluated with the Johnsonville data set allowed for an elimination of calm winds, which resulted in slightly reduced peak 1-hour and 3-hour concentrations. However, some increases in the 24-hour average concentrations were noted with this alternative. Overall, it appeared that the procedure to eliminate calm winds had little effect on peak

concentrations. At other power plant sites where the receptors are located closer to the source, and where A and B-stability has a greater effect on peak concentrations, the elimination of calm winds might be an important consideration.

As with Paradise, little additional benefit was gained by using onsite wind data in preference to airport data. This is probably because the airport site, BNA, and the Johnsonville site are similar in topography. In the diagnostic evaluation, the model using onsite wind data did show better performance over the airport model, with higher correlations and MFEs closer to zero.

The differences between the models using different dispersion schemes were again small in contrast to the differences noted with the meteorological and emission alternatives. In predicting the peak concentrations, the three basic dispersion models (PG, PG with buoyancy-induced-dispersion, and Briggs) performed about equally. The models using onsite turbulence data, however, did not perform as well as expected. The Pasquill (1976) scheme overpredicted most peak concentrations. The modeling alternatives using the Cramer and Draxler dispersion schemes gave results that were compatible to the models using the PG curves but differed substantially, on occasion, from the observations. Because the Cramer and Draxler models limited dispersion during nighttime hours, further work is needed to develop a scheme to practically estimate dispersion using routine meteorological measurements during all meteorological regimes. In this study, the PG model appeared to perform as well as the other dispersion schemes.

FINAL REMARKS

In studies of this kind, the results often suggest a need for improving modeling techniques and for obtaining more sophisticated input data. This study did not deviate from this tradition. The alternative modeling approaches used with the Johnsonville and Paradise plants yielded results that were within an order of magnitude of the peak SO_2 concentrations. Yet, further improvements are possible with more accurate source term data, more site-specific meteorological data, and more refined dispersion schemes.

The major differences in model performance resulted from differences in emission rates and, to a lesser extent, from the use of different meteorological data. The use of alternative dispersion schemes was not as significant. However, as recently outlined by Strimaitis, *et al.* (1980), efforts to improve the measurements of σ_θ and σ_ϕ (as well as other turbulence parameters) could provide a more reliable means for estimating dispersion.

The task of model evaluation in this study was especially onerous, because slight differences in predicted plume trajectories overwhelmed the statistical comparisons used to examine the alternative modeling approaches. This further substantiates the observation that the Gaussian plume dispersion model is especially sensitive to the input of wind direction. Model evaluations could perhaps be simplified by following the advice of Calder and Johnson; i.e., that each model component be separately evaluated. Otherwise, it

is difficult to compare the strengths and weaknesses of different modeling techniques. The difficulty in performing model evaluation is further compounded by a lack of field data. The availability of field data from studies such as Cinder Cone Butte, Idaho, and Kincaid, Illinois, will hopefully make the tasks of model evaluation and model improvement less formidable.

SECTION 10

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APPENDIX A
HOURLY STACK PARAMETERS

Using the data available from Paradise for 1976 and Johnsonville for 1977, the hourly values of SO_2 emission rates (Q), stack gas temperatures (T), and stack gas exit velocities (v_s) were estimated. The methodology for making these estimates is explained below.

Paradise

For the three stacks at Paradise, the following data were available:

- 1) daily coal consumption, C_d , at each stack;
- 2) sulfur analysis, S , (in percent) determined every six or seven days at each stack;
- 3) hourly power generation values for the entire plant; and,
- 4) hourly power generation values for unit three.

The first step needed to estimate the hourly SO_2 emission rates was to compute the daily average SO_2 rate at each stack. This was performed using the following equation and by assuming 100 percent conversion of sulfur to SO_2 :

$$Q_d = (64/32)(S)(C_d)$$

where 64 is the molecular weight of SO_2 , 32 is the molecular weight of sulfur, S is the average percentage sulfur content of the coal, and C_d is the amount of coal consumed daily at each stack.

The hourly SO_2 emissions were then estimated using the hourly power generation data that were available for the plant. For unit three, the following equation was used to estimate the hourly SO_2 emission rates:

$$Q(3)_h = Q(3)_d P(3)_h / P(3)_d \text{ (24 hours/1 day)}$$

where $Q(3)_h$ is the hourly emission rate for stack three, $Q(3)_d$ is the daily average emission rate for stack three, $P(3)_h$ is the hourly power generation rate for unit three, and $P(3)_d$ is the daily power generation rate for unit three.

A slightly less accurate procedure was used to estimate the hourly SO_2 emission rates for stacks one and two. Hourly power generation data were only available to this study for the combination of stacks one and two. It is believed that since both stacks are of the same height and since accurate daily coal consumption values were available for each stack, the hourly SO_2 rates can be estimated fairly accurately with the following equation:

$$Q_h = Q_d P(1\&2)_h / P(1\&2)_d \text{ (24 hours/1 day)}$$

where $P(1\&2)$ is the summed power generation values for stacks one and two and the other symbols are like those given in the previous equation.

At Paradise, values for stack gas temperatures and exit velocities were furnished for each stack by TVA for boiler capacities of 100 percent and 50 percent. The hourly capacity for each stack was estimated from the power generation values. The stack gas temperature,

T, and the exit velocity, v_s , were then computed by interpolating between their respective 100 percent and 50 percent values. When the estimated capacity was found to be greater than 100 percent, the 100 percent values for v_s and T were assumed. When the estimated capacity was found to be less than 50 percent, the 50 percent values for v_s and T were assumed.

Johnsonville

Similar procedures for estimating the hourly values of Q, v_s , and T were used for the Johnsonville stacks. The hourly generation data, however, were more limited than the Paradise data. Hourly power generation data were available for the combination of stacks one through six and for the combination of stacks seven and eight. It is believed that the hourly SO₂ emissions for the entire site were reasonably approximated since stacks one through six were the same height and stacks seven and eight were the same height. The following data were available from Johnsonville for estimating the hourly stack parameters:

- 1) daily coal consumption values for each stack;
- 2) sulfur analysis determined every six or seven days for the coal burned at each stack;
- 3) hourly power generation values for the sum of stacks one through six; and,
- 4) hourly power generation values for the sum of stacks seven and eight.

The daily average emission rates were determined with the equation used for the Paradise analysis. Then, the hourly average emission rates were computed using the available power generation data.

Values of stack gas temperature and exit velocity were furnished for the Johnsonville stacks at capacities of 100 percent, 75 percent, and 50 percent. Linear interpolation was used, like Paradise, to determine the hourly stack parameter values.

APPENDIX B
DISPERSION ALGORITHMS

BRIGGS' RURAL DISPERSION COEFFICIENTS

```
      SUBROUTINE BSYZ
C      REPLACES SUBROUTINE PGYZ, SUBROUTINE BSYZ INCORPORATES
C      BRIGGS RURAL DISPERSION COEFFICIENTS AS OUTLINED IN
C      GIFFORD'S PAPER IN NUCLEAR SAFETY (17) 1, PP. 68-86.
C
C      SUBROUTINE PROGRAMMED BY T. PIERCE FOR MASTERS
C      RESEARCH ON 5 APRIL 1981.
C
C      COMMON /MPR/ UPL,Z,H,HL,X,Y,KST,DELH,SY,SZ,RC,ISIG
C      COMMON /MPOR/ IOPT(25)
C
C      GO TO THE APPROPRIATE STABILITY CLASS
C
C      GOTO (10,20,30,40,50,60),KST
C
C      STABILITY A
C
10     SY = 220.*X/SQRT(1.+0.1*X)
      SZ = 220.*X
      GOTO70
C
C      STABILITY B
C
20     SY = 160.*X/SQRT(1.+0.1*X)
      SZ = 120.*X
      GOTO70
C
C      STABILITY C
C
30     SY = 110.*X/SQRT(1.+0.1*X)
      SZ = 80.*X/SQRT(1.+0.2*X)
      GOTO70
C
C      STABILITY D
C
40     SY = 80.*X/SQRT(1.+0.1*X)
      SZ = 60.*X/SQRT(1.+1.5*X)
      GOTO70
```

SUBROUTINE BSYZ (continued)

130

```
C
C      STABILITY E
C
50  SY = 60.*X/SQRT(1.+0.1*X)
    SZ = 30.*X/(1.+0.3*X)
    GOTO70
C
C      STABILITY F
C
60  SY = 40.*X/SQRT(1.+0.1*X)
    SZ = 16.*X/(1.+0.3*X)
C
C      CALCULATE BUOYANCY INDUCED DISPERSION IF DESIRED
C
70  IF(IOPT(4).NE.1)RETURN
    BID = DELH/3.5
    SY = SQRT(SY*SY + BID*BID)
    SZ = SQRT(SZ*SZ + BID*BID)
    RETURN
C
    END
```



```

SUBROUTINE PASQ76
C      VERTICAL DISPERSION PARAMETER VALUES, SZ, DETERMINED BY
C       $SZ = A * X ** B$  WHERE A AND B ARE FUNCTIONS OF STABILITY
C      AND THE DOWNWIND DISTANCE, X.
C      HORIZONTAL DISPERSION VALUES, SY, DETERMINED FROM
C      PASQUILL(1976):  $SY = SIGMA-A*X*F(X)$ 
C
C      PROGRAMMER: T. PIERCE
C      SIGMA-Z CALCULATIONS BASED ON PROGRAMMING OF D. B. TURNER.
C
COMMON /MPR/ UPL,Z,H,HL,X,Y,KST,DELH,SY,SZ,RC,ISIG
COMMON /MPOR/ IOPT(25)
COMMON /MOS/ SRP1,SSM1,DAY1,SINLAT,COSLAT,TDUM,T10,T110,SIGE,SIGA,
&          DSIG,JHR
DIMENSION XA(7),XB(2),XD(5),XE(8),XF(9),AA(8),BA(8),AB(3),
&          BB(3),AD(6),BD(6),AE(9),BE(9),AF(10),BF(10)
DATA XA/.5,.4,.3,.25,.2,.15,.1/
DATA XB/.4,.2/
DATA XD/30.,10.,3.,1.,.3/
DATA XE/40.,20.,10.,4.,2.,1.,.3,.1/
DATA XF/60.,30.,15.,7.,3.,2.,1.,.7,.2/
DATA AA/453.85,346.75,258.89,217.41,179.52,170.22,158.08,122.8/
DATA BA/2.1166,1.7283,1.4094,1.2644,1.1262,1.0932,1.0542,0.9447/
DATA AB/109.30,98.483,90.673/
DATA BB/1.0971,0.98332,0.93198/
DATA AD/44.053,36.650,33.504,32.093,32.093,34.459/
DATA BD/0.51179,0.56589,0.60486,0.64403,0.81066,0.86974/
DATA AE/47.618,35.420,26.970,24.703,22.534,21.628,21.628,23.331,
&          24.26/
DATA BE/0.29592,0.37615,0.46713,0.50527,0.57154,0.63077,0.75660,
&          0.81956,0.8366/
DATA AF/34.219,27.074,22.651,17.836,16.187,14.823,13.953,13.953,
&          14.457,15.209/
DATA BF/0.21716,0.27436,0.32681,0.41507,0.46490,0.54503,0.63227,
&          0.68465,0.78407,0.81558/
XY = X
GOTO (10,40,70,80,110,140), KST
C      STABILITY A
10  IF (X.GT.3.11) GO TO 170
    DO 20 ID=1,7
    IF (X.GE.XA(ID)) GO TO 30
20  CONTINUE
    ID = 8
30  SZ = AA(ID)*X**BA(ID)
    GO TO 190

```

```
C      STABILITY B
40    IF (X.GT.35.) GO TO 170
      DO 50 ID=1,2
      IF (X.GE.XB(ID)) GO TO 60
50    CONTINUE
      ID=3
60    SZ=AB(ID)*X**BB(ID)
      GO TO 190
C      STABILITY C
70    SZ=61.141*X**0.91465
      GO TO 190
C      STABILITY D
80    DO 90 ID=1,5
      IF (X.GE.XD(ID)) GO TO 100
90    CONTINUE
      ID=6
100   SZ=AD(ID)*X**BD(ID)
      GO TO 190
C      STABILITY E
110   DO 120 ID=1,8
      IF (X.GE.XE(ID)) GO TO 130
120   CONTINUE
      ID=9
130   SZ=AE(ID)*X**BE(ID)
      GO TO 190
C      STABILITY F
140   DO 150 ID=1,9
      IF (X.GE.XF(ID)) GO TO 160
150   CONTINUE
      ID=10
160   SZ=AF(ID)*X**BF(ID)
      GO TO 190
170   SZ=5000.
C      SIGMA-Y CALCULATIONS, MODIFIED ON 22 SEPTEMBER 1981
C      WITH SUGGESTIONS MADE BY J. IRWIN.
190   FX = 1. + SQRT(X/2.5)
      SY = SIGA * 1000. * X / FX
C      COMPUTE BUOYANCY INDUCED DISPERSION
      BID = DELH/3.5
      SZ = SQRT(SZ*SZ+BID*BID)
      IF (SZ.GT.5000.) SZ = 5000.
      RETURN
C
      END
```

DRAXLER (1976)

```

SUBROUTINE DRAX
C   CALCULATES SIGMA-Y AND SIGMA-Z USING MEASUREMENTS OF
C   SIGMA-THETA AND SIGMA-PHI.
C   REFERENCE: DRAXLER(1976)
C
C   PROGRAMMER: T. PIERCE      30 OCTOBER 1981
C
COMMON /MPR/ UPL,Z,H,HL,X,Y,KST,DELH,SY,SZ,RC,ISIG
COMMON /MOS/ SRP1,SSM1,DAY1,SINLAT,COSLAT,TDUM,T10,T110,SIGE,SIGA,
&           DSIG,JHR
C
C   X IN KM, T = 1000S
C
FY=1./(1.+0.9*SQRT(X/UPL))
SY=SIGA * 1000. * X * FY
C
C   STABLE CASE, ALLOW ESSENTIALLY NO VERTICAL SPREADING
C
IF (KST.GE.4) THEN
  IF (KST.EQ.4) THEN
    IF (DSIG.NE.DAY1) CALL SUN
    IF (JHR.GE.SRP1.AND.JHR.LT.SSM1) GOTO10
  ENDIF
  FZ=0.
  ELSE
C   T = 500 SEC
C
10  FZ=1./(1.+0.9*SQRT(2.*X/UPL))
    ENDIF
    SZ=SIGE * X * 1000. * FZ
C
C   BOUYANCY INDUCED DISPERSION
C
  BID = DELH/3.5
  SZ = SQRT(SZ*SZ + BID*BID)
  RETURN
  END

```

SUBROUTINE CRAM

INCORPORATES THE EQUATIONS PRESENTED BY CRAMER(1976) TO
ESTIMATE SIGMA-Y AND SIGMA-Z FROM ON-SITE MEASUREMENTS
OF SIGMA-A AND SIGMA-E.

PROGRAMMER: TOM PIERCE 30 OCTOBER 1981
METEOROLOGIST (FROM NOAA)
ENVIRONMENTAL OPERATIONS BRANCH
U.S. ENVIRONMENTAL PROTECTION AGENCY
RESEARCH TRIANGLE PARK, NC 27711

BASIC REFERENCE:

CRAMER, H. (1976)
'IMPROVED TECHNIQUES FOR MODELING THE DISPERSION FROM
TALL STACKS' 7TH NATO/CCMS MEETING, 7-10 SEPTEMBER 1976,
ARLIE, VA, PP. 731-780.

OTHER REFERENCES:

IRWIN, J. (1978)
SCHEME FOR ESTIMATING DISPERSION PARAMETERS AS A
FUNCTION OF RELEASE HEIGHT, EPA-600/4-79-062, U.S.EPA,
RESEARCH TRIANGLE PARK, NC, PP. 68.

PASQUILL, F. (1976)
POSSIBLE REQUIREMENTS FOR CHANGE IN THE TURNER WORKBOOK
VALUES, EPA-600/4-76-030B, U.S. EPA, RESEARCH TRIANGLE
PARK, NC, PP. 53.

COMMON AND DIMENSION STATEMENTS---

COMMON /MOS/ SRP1,SSM1,DAY1,SINLAT,COSLAT,TDUM,T10,T110,SIGE,SIGA,
DSIG,JHR
COMMON /MPR/ UPL,Z,H,HL,X,Y,KST,DELH,SY,SZ,RC,ISIG
DIMENSION P1KST(6),P2KST(6)

INPUT PARAMETERS:

DELH PLUME RISE (M)
H EFFECTIVE HEIGHT (M)
KST PG STABILITY CLASS
SIGA STANDARD DEVIATION OF THE MEASURED HORIZONTAL WIND
DIRECTIONS AS MEASURED AT HEIGHT ZMA (IN RADIANS)
SIGE STANDARD DEVIATION OF THE MEASURED VERTICAL WIND
DIRECTIONS AS MEASURED AT HEIGHT ZME (IN RADIANS)
T10 ON-SITE 10M AMBIENT AIR TEMPERATURE (KELVIN)
T110 ON-SITE 110M AMBIENT AIR TEMPERATURE (KELVIN)
X DOWNWIND DISTANCE (KM)


```
C---INITIALIZATIONS---
C
C      HEIGHT ADJUSTMENTS AS A FUNCTION OF STABILITY FOR
C      SIGMA-E (P1KST) AND SIGMA-A (P2KST)
C
C      DATA P1KST/.08,.08,.05,.0,-.45,-.65/,
&      P2KST/-.07,-.07,-.10,-.15,-.35,-.55/
C
C      AMBIENT AIR TEMPERATURE
C
C      DATA TA /293./
C
C      XRY - DISTANCE OF RECTILINEAR PLUME EXPANSION (50M)
C
C      XRY = 50.
C
C      CONVERT DISTANCE TO METERS
C
C      XM = X * 1000.
C
C      SET TA TO T10 IF MEASUREMENT IS AVAILABLE
C
C      IF(T10.GT.0.) TA = T10
C
C      DTDZ: 110M - 10M TEMPERATURE (LAPSE RATE)
C
C      IF(T110.GT.0. .AND. T10.GT.0.) THEN
C          DTDZ=(T110-T10) * .01
C      ELSE
C          DTDZ=-1.
C      ENDIF
C
C      MEASUREMENT HEIGHT (M) FOR SIGA (ZMA) AND SIGE (ZME)
C
C      ZMA=110.
C      ZME=110.
C---CALCULATIONS---
C
C      ADJUST SIGMA-E UP TO PLUME HEIGHT (H)
C
C      P1 = P1KST(KST)
C      HFACE = H/ZME
C
C      USE CRAMER(1976) EQUATION 29, P.755
C
C      IF(KST.LE.4) THEN
C          RATIO=H/HL
```


SUBROUTINE CRAM (continued)

136

```
C
C      TEST FOR INCREASE OF SIGMA-E WITH HEIGHT, LIMIT INCREASE
C      OF SIGMA-E TO LOWER 50% OF HL, FROM IRWIN(1978)
C
      IF(RATIO.GT..25)HFACE=.25*HL/ZME
      ENDIF
C
C      CRAMER(1976) EQUATION 29, P. 755
C
      SGPRM = SIGE * (HFACE)**P1
C
C      CHECK FOR LOFTING TYPE OF CONDITION BY LOOKING AT THE
C      STABILITY CLASS. IF D-NIGHT AND STABLE, THEN SUPPRESS
C      AMBIENT TURBULENCE IN THE VERTICAL. THE ONLY MECHANISM
C      FOR VERTICAL SPREADING WILL BECOME BUOYANCY INDUCED DISP.
C
      IF(KST.EQ.4)THEN
        IF(DSIG.NE.DAY1)CALL SUN
        IF((JHR.LT.SRP1).OR.(JHR.GT.SSM1))SGPRM=.001
      ENDIF
      IF(KST.GT.4)SGPRM=.001
C
C      ADJUST SIGMA-A TO PLUME HEIGHT (H)
C
      P2 = P2KST(KST)
C
C      CRAMER(1976) EQUATION 28, P.752
C
      SGAPRM = SIGA * (H/ZMA)**P2
C
C      CALCULATE PLUME ENHANCEMENT, FROM CRAMER(1976) EQUATION 5,
C      P.739, SIMILAR TO PASQUILL'S BUOYANCY INDUCED DISPERSION
C
      BID = DELH/4.3
C
C      CALCULATE THE STABILIZATION DISTANCE, XR
C      CRAMER(1976) EQUATION 6, P.740
C
      XR = 10.*(H-DELH)
      IF(KST.GT.4)THEN
        IF(DTDZ.LE.0.)THEN
          DTDZ=.02
          IF(KST.GE.6)DTDZ=.035
        ENDIF
        XRALT=UPL*3.141593/SQRT(9.80616*DTDZ/TA)
C
C      (STABILITY) S=G*DTDZ/T (DTDZ=LAPSE RATE)
C
      IF(XRALT.LT.XR)XR=XRALT
      ENDIF
```

```
C
C      CALCULATE SIGMA-Z (CRAMER, 1976 EQUATION 11, P.742)
C
C      FIRST CALCULATE VIRTUAL DISTANCE, XZ USING
C      CRAMER(1976) EQUATION 12, P.742
C
      XZ=0.
      XRCHK=BID/SGEPRM
      IF (XRCHK.GE.XR) XZ=XRCHK-XR
      SZ=SGEPRM*(XM+XZ)
C
C      IF LOFTING CONDITION, THEN SET SZ=BID
C
      IF (SGEPRM.EQ..001) SZ=BID
C
C      LIMIT SIGMA-Z TO 5000M OR .8 HL IN UNSTABLE/NEUTRAL
C
      IF (SZ.GT.5000.) SZ=5000.
      IF (KST.LE.4) THEN
        EHL=.8*HL
        IF (SZ.GT.EHL) SZ=EHL
      ENDIF
C
C      CALCULATE SIGMA-Y WITH CRAMER(1976) EQUATION 9, P.741
C
C      FIRST CALCULATE THE VIRTUAL DISTANCE, XY WITH
C      CRAMER(1976) EQUATION 10, P.742
C
      XRYCHK=BID/SGAPRM
      IF (XRYCHK.LE.XRY) THEN
        XY=XRYCHK-XR
      ELSE
        XY=0.9*XRY*((XRYCHK/XRY)**1.11111)-XR+XRY*0.1
      ENDIF
      IF (XY.LT.0.) XY=0.
C
      SY=SGAPRM*XRY*((XM+XY-XRY*.1)/(.9*XRY))**0.9
      RETURN
      END
```